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# TWO-DIMENSIONAL AVALANCHE BREAKDOWN IN Pt-Si SCHOTTKY BARRIER DIODES

**Applied Electronic Research Corporation** 

David P. Kennedy



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Under Contract No. F19628-77-C-0220 Applied Electronic Research Corporation undertook the development of a two-dimensional computer model for calculating avalanche breakdown in a Pt-Si Schottky barrier diode. A principal objective of this program was to develop such a computer program, and make the sourcecode and operational data available to other workers in the field. Further, as a means to verify the applicability of this program junction, breakdown computations were to be undertaken throughout a wide range of physical parameters and ambient temperatures. DD 1 JAN 73 1473 UNCLASSIFIED

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### Evaluation

The Final Report on Two-Dimensional Avalanche Breakdown in Pt-Si
Schottky Barrier Diodes represents a half-man year effort over 12
months to calculate numerically the breakdown characteristics of Schottky barrier diodes on p-type silicon. The results clearly indicate that avalanche breakdown is not the appropriate mechanism to explain the experimentally observed reverse characteristics of these diodes; a far closer agreement is achieved with calculations based on a one carrier multiplication process. Preliminary considerations also indicate that it is inappropriate to apply Schottky barriers on n-type theoretical treatment to Schottky barrier on p-type diodes. In the former case tunneling may be an important leakage component. The findings of this contract have important applications to Schottky barrier based 3-5 micrometer infrared detector staring arrays as well as low temperature electronics.

SVEN A. ROOSILD Project Engineer

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### Summary and Major Results

A two-dimensional computer model has been developed for avalanche breakdown in a Pt-Si Schottky barrier diode, assuming either p-type or n-type semiconductor material. After completing this model, comparisons between experiment and theory suggested a need to undertake model modifications; assuming carrier multiplication processes other than a classical Townsend avalanche processes. Those modifications were undertaken and completed. As a consequence, two different computer models are being made available: first, a model assuming classical Townsend avalanche breakdown and, second, a model assuming one-carrier multiplication within a pt-Si space-charge layer.

Both of these computer programs utilize finite-difference methods within a two-dimensional grid containing non-equal spacing. Thereby, substantial computational accuracy is obtained throughout regions of the structure containing large values of electric field and a significant level of carrier multiplication. User options permit adequate variation of the geometrical and physical parameters in this model to make it valuable tool for fundamental studies associated with two-dimensional Schottky barrier operation.

Computational techniques have been employed that appear to reduce overall computation time to a satisfactory level. Specifically, these computer programs are designed to undertake a search for the carrier trajectory producing a maximum of carrier multiplication, at a given applied voltage; in contrast with undertaking a calculation of all carrier trajectories and their respective levels of carrier multiplication. Further, the system of finite difference equations generated during a given two-dimensional solution of Poisson's equation are solved using efficient spacematrix techniques. Stone's method is applied in an iterative loop for calculating the potential distribution throughout the space-charge layer of a Pt-Si Schottky barrier diode.

Avalanche breakdown calculations were undertaken for physical parameters typical of devices being fabricated in laboratory experiments. Important differences were observed between experiment and theory: the

calculated breakdown voltage was higher than observed in the laboratory, and the calculated avalanche breakdown process was substantially more abrupt. It was these results that suggested a change in the model for carrier multiplication—to a one-carrier process. This model modification did, indeed, produce a soft breakdown characteristic and better agreement with experiment.

A one-carrier multiplication process yields a reverse current that increases nearly exponentially with voltage. It was found that some laboratory devices do indeed exhibit an exponential current/voltage relation throughout a substantial range of reverse current. Unfortunately, little inference can be drawn from this observation; theory also predicts that carrier tunneling at the metal/Si interface would exhibit a similar current-voltage relation. For this reason it is suggested that the reverse current observed in a p-type Pt-Si diode does not exhibit those characteristics expected from an avalanche breakdown process. Instead, it is suggested that this reverse current could arise from either one-carrier multiplication within the space-charge layer or from carrier tunneling at the metal-Si interface.

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### CHAPTER I

A Two-Dimensional Computer Model for Avalanche Breakdown in Schottky Barrier Diodes

### 1.0 Introduction

Schottky barriers formed with metal-silicide compounds in contact with silicon are known, under some conditions, to exhibit "soft" reverse breakdown characteristics. That is to say the reverse current is observed to increase gradually, rather than abruptly, as the barrier is biased in the reverse direction. This phenomenon is observed, for example, with platinum-silicide Schottky barriers, using p-type silicon and operated at liquid nitrogen temperature (77° K).

Possible causes for this soft breakdown phenomenon are: First, unlike barriers formed by the juncture of a pure metal (such as gold) in contact with silicon, the kinetics of the growth of a metal-silicide compound produces a metal-silicide region which penetrates into the silicon substrate in a manner similar to a shallow diffusion [1]. Thus, two-dimensional mechanisms exist, wherein high electric fields may develop at the periphery of the barrier causing breakdown to occur, due to avalanche multiplication. Second, mechanical stress at the interface [2, 3] can enhance this breakdown phenomenon. Third, the existence of surface states could lead to enhanced breakdown. Fourth, quantum mechanical tunneling of carriers through the potential barrier formed at the metal-silicide-silicon interface also represents possible cause of soft breakdown.

Work performed under this program addressed the following tasks:

- A.--Develop a two-dimensional computer solution for Poisson's equation, using boundary conditions that include a metal-silicide Schottky barrier on p-type silicon. Further, the surface of this structure is bounded by a thermal oxide containing positive charges, accounting for oxide-silicon interface states.
- B.--Develop a two-dimensional computer solution for the Townsend carrier multiplication process.
- C.--Calculate the breakdown voltage of a Schottky barrier on p-type silicon as a function of the following parameters:

- 1. Barrier height (from 0.25 ev to 0.35 ev)
- 2. Resistivity (from 1.0 to 100 chm cm)
- 3. Ox/Si interface charge  $(10^{-7} \text{ to } 10^{-9} \text{ coul:/cm}^2)$
- 4. Temperature (77°K to 300°K)
- D.--Extend the above model to permit the treatment of N-type silicon structures of the same type described in A, above.

### 2.0 Description of the Computer Model

The computer model treats either p-type or N-type substrate materials, the distinction being determined through a "flag" incorporated in the input data parameters in a manner to be clarified in a later subsection. It is capable of treating arbitrary doping densities and temperatures, also specified as input parameters. Considerable flexibility is also incorporated insofar as the geometry is concerned.

### 2.01 Basic Geometry

Figure 1 illustrates the geometry assumed in this computer model. A rectangular region is defined, containing a metal-silicide region of constant potential (i.e. it is treated as if it were a metal), having the value (V<sub>bi</sub> + V). Here V<sub>bi</sub> is the "built-in" equilibrium potential between the two regions, while V is the externally applied reverse bias voltage. This metal-silicide region is considered to be a rectangle, with dimensions  $X_m$  by  $Y_m$ , with a circular lower right corner. The overall rectangular region extends to the right of and below the metal-silicide region by 1.25 depletion widths; thereby, we are assured that all boundaries are located in charge-neutral substrate material. Our definition of a "depletion width" hinges upon the geometric parameters  $X_m$ ,  $Y_m$ , and  $r_m$ . In the event that all three are equal, and if the silicon-oxide surface charge Q is zero, then a one-dimensional depletion solution of Poisson's equation (in cylindrical coordinates) is used to establish the required width. If, instead, any of these conditions are violated (thereby destroying the circular symmetry) planar depletion theory is applied to determine the depletion layer width.

The left border (extending below the metal-silicide region) is treated as a symmetry plane along which the normal derivative of the electrostatic potential is set to zero. A similar boundary is used for the upper border (extending to the right of Pt-Si region), except that the normal derivative

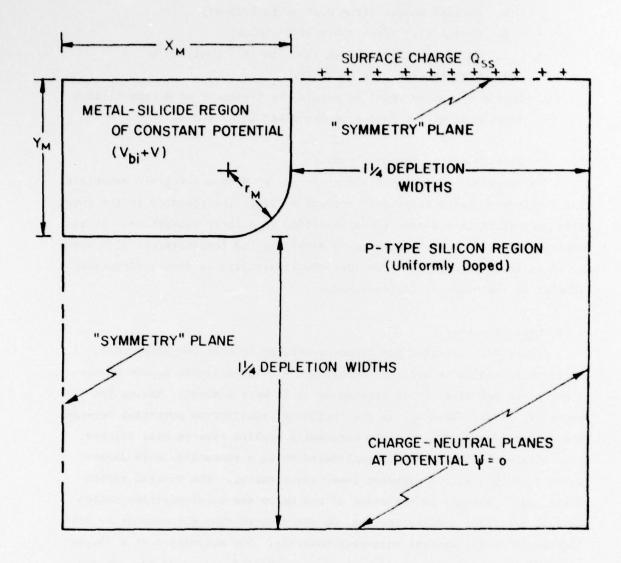


Fig. 1
Geometrical Model used in this Computer Program

of electrostatic potential becomes discontinuous when the surface charge  $\mathbf{Q}_{_{\mbox{\footnotesize{\bf SS}}}}$  is nonzero.

This computer model deals with a graded lattice of mesh points over-layed upon the foregoing rectangular region. Lattice grading is automatically implemented by a part of this computer program. Such grading has been designed to make the density of mesh points highest in the vicinity of the metal-silicide-silicon interface; thereby enhancing the accuracy of the finite-differences algorithms throughout the region where avalanche multiplication occurs. Figure 2 illustrates such a graded lattice for the case where  $X_m = Y_m$ , using an array of 31 by 31 mesh points.

### 2.02 Normalized Variables

With a few exceptions which are clearly flagged by COMMENT statements, this computer model deals with normalized variables. These variables are defined in terms of the following normalization parameters:

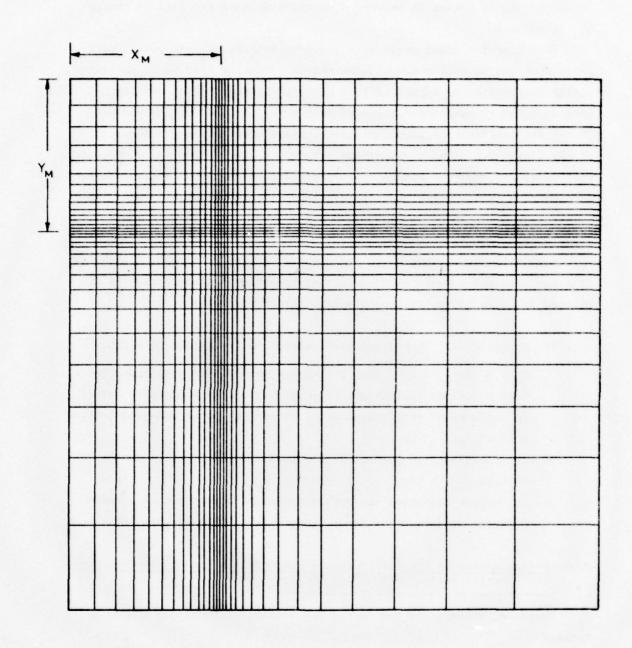
- Distances are normalized with respect to the depletion width,  $W_{D} = \sqrt{2E(V_{bi} + V) / (qN_{a})}, \text{ obtained from planar depletion theory.}$  Here  $N_{a}$  is the ionized acceptor density at temperature T. (This is replaced by the ionized donor density  $N_{d}$ , when modeling N-type structures.)
- 2) The electrostatic potential is normalized with respect to the voltage ( $V_{\rm bi}$  + V).
- 3) All charge densities are normalized with respect to the ionized acceptor density  $N_{\rm a}$  or donor density  $N_{\rm d}$ , as the case may be.

## 2.03 Determination of the Electrostatic Potential $\psi$ , and the corresponding Electric Field Components E $_{\rm X}$ & Ey.

Expressed in terms of the normalized variables, Poisson's equation becomes:

$$\nabla^2 \Psi = 2[1 + n - p] = Q \tag{1.01}$$

where  $\psi$  is the electrostatic potential, while p and n are the normalized hole and electron densities, respectively. The former, in dimensionless variables, is related to  $\psi$  through the Boltzmann relationship:



 $$\operatorname{Fig.} 2$$  Illustration of Lattice Grading Established in Subroutine GRID

$$p = \exp(-q[V_{bi} + V] \psi/kT),$$
 (1.02)

which implies nondegenerate doping of the substrate material. The latter is similarly expressed by:

$$n = n_i^2 \exp(q[V_{bi} + V) \psi - V]/kT), \qquad (1.03)$$

where n, is the normalized intrinsic density at temperature T.

Equations (1.02) and (1.03) are based upon an approximation which ignores gradients in the hole and electron quasi-Fermi potentials; both are assumed to be independent of X and Y throughout the silicon substrate region. This assumption, widely used in p-n junction breakdown calculations, is justified by the success of such calculations in predicting breakdown voltages in excellent agreement with experimental results. When the reverse bias voltage V is nonzero, (1.03) implies that the electron quasi-Fermi potential differs from that for holes by the value V. Note that (1.03) correctly gives  $n = n_1^2 \exp(qV_{bi}/kT)$  at the metal-silicidesilicon interface, where  $\Psi$  has the value of unity in normalized units. Further, (1.02) and (1.03) correctly yield the mass action law,  $pn = n_1^2$ , under equilibrium conditions (i.e. when V = 0).

The nonlinear problem posed by (1.01) through (1.03) is solved iteratively by the computer model. An initial "guess" is first obtained for  $\psi$ , using depletion theory. Equations (1.02) and (1.03) then yield initial estimates for p and n at each lattice mesh point, and therefore for the right hand side of (1.01). That equation, when expressed in finite-difference form for a lattice where dimensions are m by n, transforms into m times n coupled linear equations for  $\psi$  at each mesh point. Expressed in matrix form, the resultant matrix is very sparse, having only five non-zero diagonals. Stone's iterative matrix factorization method [4] is then utilized to obtain a revised estimate for  $\psi$  at each of the mesh points. Then (1.02) and (1.03) provide corresponding revised estimates for p and n. This procedure is applied repetitively until self-consistent solutions of (2.01) through (2.03) result. The implementation of this iterative process utilizes Grummel's algorithm [5], as modified by Sutherland [6], to enhance its convergence.

With a self-consistent solution of Poisson's equation in hand, the normalized electric field components  $\mathbf{E}_{\mathbf{x}}$  and  $\mathbf{E}_{\mathbf{v}}$  are obtained using finite

differences. These electric field components are stored two arrays, for subsequent use in calculating the free carrier trajectories, and the Townsend multiplication integrals.

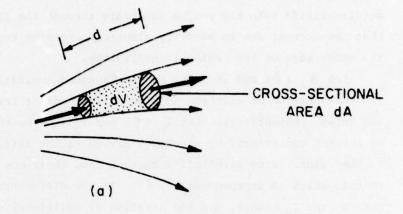
### 2.04 Determination of the Two-Dimensional Free Carrier Trajectories

The evaluation of the Townsend multiplication integrals requires knowledge of the curvilinear trajectories traced out by the charge carriers involved in that process. Since significant multiplication occurs only in regions where the electric field (unnormalized) exceeds 2 x 10  $^5$  volts/cm, the effects of diffusion forces are negligible in comparison with the electrostatic forces acting upon said carriers. Thus, the resultant velocity vector  $\vec{\mathbf{v}}$  is colinear with the electric field vector  $\vec{\mathbf{E}}$  ( $\vec{\mathbf{v}}=\boldsymbol{\mu}$   $\vec{\mathbf{E}}$  in normalized units, with  $\boldsymbol{\mu}$  the normalized carrier mobility.) As a result, the paths of the carriers coincide everywhere with electrostatic flux lines, regardless of the numerical value of their mobility. Therefore, in determining those paths, it is sufficient to set the normalized mobility equal to unity, and this is what is done in the computer model.

The two-dimensional equations of motion are solved using a subprogram which implements the Adams-Bashforth-Moulton predictor-corrector algorithm [1] with time of flight as the independent variable. This subprogram provides for automatic interval halving (and doubling), controlled by monitoring the difference between the predicted and corrected values of the charge carrier's position as a function of the time of flight.

### 2.05 Determination of the Townsend Multiplication Ratio M

Figure 3 depicts a region in which two-dimensional Townsend multiplication processes are in progress. Part (a) of that figure sketches a few curvilinear streamlines, and singles out a small differential volume dV, where "sidewalls" coincide with the streamlines, and the ends are perpendicular to the streamlines. Although such streamlines for two-dimensional flow may converge or diverge, conservation of electric current requires that the net current entering one end of such a differential volume must equal the net current leaving it through the other end. From such an argument it is concluded that the Townsend multiplication process can be treated as a one-dimensional problem in the spacial coordinate  $\xi$ , which is singly curvilinear distance measured along such a streamline. Fart (b) of the figure depicts this one-dimensional problem in  $\xi$ .



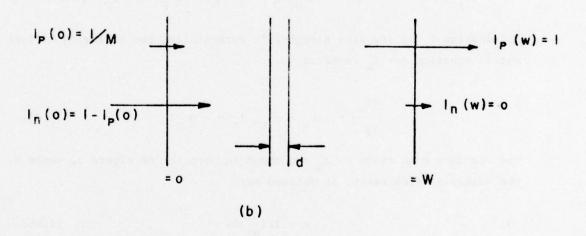


Fig. 3
Stream Lines in A Semiconductor Material
a) Two Spatial Dimensions
b) One-Dimension Approximation

Next we discuss multiplication in terms of p-type material, with the understanding that an interchange of subscripts p and n will make the results applicable to n-type material as well. We assume that the multiplication process is initiated by the injection of majority holes from the metal-silicide into the p-type substrate through the plane  $\xi = 0$ , and that the current due to minority electrons crossing the plane  $\xi = 0$  at the other edge of the region is negligible.

Let  $\alpha_n$  ( $\xi$ ) and  $\alpha_p$  ( $\xi$ ) be the Townsend ionization coefficients for the creation of electron-hole pairs (per cm) of travel of electrons and holes, respectively. Let  $I_n$  ( $\xi$ ) and  $I_p$  ( $\xi$ ) be the local components of current contributed by electrons moving to the left and holes moving to the right. From Kirchhoff's current law, their sum is the total current I, which is independent of  $\xi$ . In the differential distance d  $\xi$ , both  $I_n$  and  $I_p$  change, due the creation of additional electron-hole pairs:

$$dI_{p}(\xi) = dI_{n}(\xi) = (\alpha_{n}(\xi) I_{n}(\xi) + \alpha_{p}(\xi) I_{p}(\xi)]d\xi$$
 (1.04)

Eliminating  $\mathbf{I}_{p}$  by invoking Kirchhoff's current law, the following differential equation for  $\mathbf{I}_{n}$  results:

$$\frac{dI_n}{d\xi} + (\alpha_n - \alpha_p) I_n = -\alpha_p I \qquad (1.05)$$

The boundary conditions on  $I_n$  are shown in part (b) of Figure 3, where M, the multiplication ratio, is defined as:

$$M = I/I_{p} (0)$$
 (1.06)

The solution of (1.05) which satisfies those boundary conditions leads to the following relationship for M:

$$M = \begin{cases} \frac{1}{1 - \int_{0}^{w} \alpha_{p}(\xi) \exp\left\{\int_{0}^{\xi} \left[\alpha_{p}(\xi') - \alpha_{p}(\xi')\right] d\xi'\right\} d\xi} \end{cases} (1.07)$$

Inspection of this result reveals that M approaches an infinite value as the integral expression in the denominator approaches unity. Since the  $\xi$ -dependence of  $\alpha_n$  and  $\alpha_p$  in the integrand depends upon the magnitude and  $\xi$ -dependence of the electric field E which, in turn, depends upon the applied reverse bias voltage V, there will always exist a value for the latter which will cause M to approach infinite values. This is the condition known as avalanche breakdown, and the value of V which causes it is the reverse breakdown voltage. As will be seen in the next chapter, where the results obtained with the computer model are discussed, this breakdown phenomenon takes on a "soft" appearance in the reverse I-V characteristic curve only when the radius of curvature  $r_m$  of the metalsilicide region is very small.

The derivation leading to (1.07) for M assumed a two-carrier multiplication process wherein both electrons and holes contribute to the avalanche mechanism. For silicon, however, experimental data for the ionization coefficients  $\alpha_n$  and  $\alpha_p$  as a function of the electric field E show that  $\alpha_p$  is more than an order of magnitude less than  $\alpha_n$ , except for very large electric fields [8]. Thus, electrons, once created by impact ionization, are much more effective than holes in creating additional electron-hole pairs. This leads one to question whether or not a "soft" breakdown characteristic might result due to single carrier multiplication, wherein only electrons are responsible for the creation of additional electron-hole pairs. In other words, what would result if  $\alpha_D$  ( $\xi$ ) were assumed to be zero?

Inspection of (1.07) shows that merely setting  $\alpha_p$  ( $\xi$ ) to zero will not work in this particular equation; no multiplication is obtained (M = 1). This conclusion arises from the fact that when  $\alpha_p$  ( $\xi$ ) = 0 (in the form of  $I_p$  (0) in the boundary conditions, with  $I_n$  (w) = 0) only holes can initiate the avalanche process. Setting  $\alpha_p(\xi)$  = 0 and retaining  $I_n$  (w) = 0, implies than an electron-hole pair can never be created, and since only electrons so created are assumed to contribute to the creation of additional electron-hole pairs, unity values of M are the natural consequence. The assumption of negligible electron current at  $\xi$  = W must be removed if there is to be any resultant multiplication when  $\alpha_p$  ( $\xi$ ) = 0.

To explore the implications of single carrier multiplication due to electrons alone, insofar as "soft" breakdown is concerned, we elected to

treat the extreme case in which only electrons initiate the avalanche process, and cause the creation of additional electron-hole pairs. This is achieved by redefining M to be:

$$M = I/I_{p}$$
 (w) (1.08)

$$I_{p}(0) = 0$$

$$I_{n}(0) = I$$

$$I_{p}(w) = I - I_{n}(w).$$
(1.09)

Then  $\alpha_{\rm p}$  ( $\xi$ ) is set to zero in (1.05). The resulting expression for M becomes:

$$M = \exp\left\{\int_0^W \alpha_n(\xi) d\xi\right\}$$
 (1.10)

This result clearly exhibits a "soft" breakdown characteristic inasmuch as M approaches infinite values only as the integral in (1.10)
does so also. There is no finite reverse bias voltage V leading to an
infinite current. Such a conclusion is not surprising; it was precisely
such a conclusion that encouraged Townsend to postulate two-carrier multiplication.

There is a problem with this result, and this problem is associated with the redefinition of M (compare (1.06) with (1.09)). In a hole initiated multiplication process the reverse saturation current of the Schottky barrier is clearly a consequence of space-charge generated holes that move to the p-type substrate material. In the latter case, it is the current due to minority electrons flowing from the p-substrate to the metal-silicide. The former is many orders of magnitude larger than the latter, especially at reduced temperatures. At  $77^{\circ}$ K, for example, the intrinsic electron density in silicon is  $5.22 \times 10^{-20}$  cm<sup>-3</sup>. With an acceptor density of  $10^{15}$  cm<sup>-3</sup>, the corresponding equilibrium minority electron density in the charge-neutral substrate is calculated to be  $2.73 \times 10^{-54}$ /cm<sup>3</sup>. Thus, in Fig. 3, the minority electron current crossing the plane  $\xi = W$  should be a negligible factor in contributing to the reverse I-V characteristic.

From the foregoing discussion it is evident that single carrier multiplication, due to electrons, is an implausible mechanism in an ideal semiconductor structure. If, instead, substantial lattice damage exists (micro-cracks, strain, etc.), electron/hole generation could take place, and such damage could represent a significant source for electrons. For this reason (1.10) has been also implemented in the present computer model, and this expression leads to results differing from (1.07).

The computer model functions as follows when evaluating the above expressions for M. A search is first made to ascertain the location of the maximum electric field along the metal-silicide-silicon interface. Three trajectories are then determined, the middle one initiating at the point of maximum E, the other two bracketing it. Equation (1.07) is next evaluated along all three paths, and a test is made to ascertain which of the three produces maximum M. If not the middle path, the pattern of three paths is shifted left or right along the interface, accordingly, and the process is repeated until the middle path produces a maximum M for a given applied voltage V. In the special case that the geometry under study has circular symmetry (i.e.  $X_m = Y_m = r_m$ , and  $Q_{SS} = 0$ ), this trial and error search procedure is bypassed. (The symmetry then assures that all paths will produce the same M, and only a single trajectory need be treated. The one selected is that which initiates in the diagonal plane of symmetry.)

Two versions of the subprogram for evaluating the breakdown phenomenon have been developed. The first subprogram, which is designed to find a voltage V producing an infinite value of M, requires a substantially greater computation time. The second subprogram is designed to provide data for plotting M versus V.

In the first version, an assumed applied voltage V is varied, using an iterative process, until the two-carrier multiplication factor M changes sign. This change of sign signifies that the breakdown voltage has been bracketed. During iteration the two-dimensional potential distribution, and the electric field distribution, are scaled with the revised estimates for V, in accordance with their dependency upon V from planar depletion theory. This scaling is done to avoid repeated new solutions of Poisson's equation, and repeated new trajectory calculations. Once having "zeroed" in on a correct V, however, the entire procedure is then repeated iteratively. New self-consistent solutions for the potential and electric

field are generated, and new trajectory calculations are undertaken to find a path of maximum M and a revised estimate for V. This iterative process is continued until the most recent estimate of the breakdown voltage is within a specified percentage of its previous value.

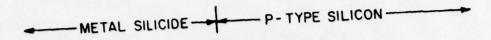
With the second version of this computer program, the applied voltage V is varied through a given range, in given increments, and the corresponding values of M (using both (1.07) and (1.10) are determined and tabulated. This version is much more useful for exploring "soft" breakdown tendencies, supplying as it does direct information for plotting curves showing M versus V.

A simplified version of (1.07) is used for avalanche breakdown calculations. In this version (1.07)  $\alpha_n$  and  $\alpha_p$  are assumed equal, having a dependence upon electric field as determined by Kennedy and O'Brien [9], and found to produce results in good agreement with experiment for a wide variety of silicon p-n junction devices. The Kennedy-O'Brien value of  $\alpha$ , for room temperature, is corrected for the specified operating temperature T fitting to the theoretical results of Baraff [10], as discussed by Crowell and Sze [11]. The second version of this computer program, discussed above, utilizes Crowell and Sze's formulas directly to obtain estimates for both  $\alpha_n$  and  $\alpha_p$  for use in (1.07) and (1.10). As a consequence of these differences, the two approaches yield slightly different estimates for the voltage leading to avalanche breakdown.

### 2.06 Calculation of the Temperature-Dependent Parameters

Figure 4 illustrates the energy band diagram (in electron volts) for a Schottky barrier on p-type silicon, and defines the intrinsic and extrinsic Fermi levels  $\mathbf{E_i}$  and  $\mathbf{E_f}$ , the valence and conduction band edge energies  $\mathbf{E_v}$  and  $\mathbf{E_c}$ , the energy gap  $\mathbf{E_g}$ , the acceptor impurity level  $\mathbf{E_a}$ , (all referred to the charge-neutral substrate region), as well as the Schottky barrier height  $\phi_B$  and the "built-in" potential difference  $\mathbf{V_{bi}}$ . The interrelationship between these fundamental parameters, and the dependence of the intrinsic and extrinsic majority hole densities upon them, are sensitive to temperature (in some instances dramatically) as well as to the doping density. These dependencies are taken into account in a subprogram of the computer model in the manner next to be described.

a) Energy Gap. -- The energy gap E<sub>g</sub> is slightly dependent upon temperature. The following formula is an empirical fit to Figure 10.2 of [12]:



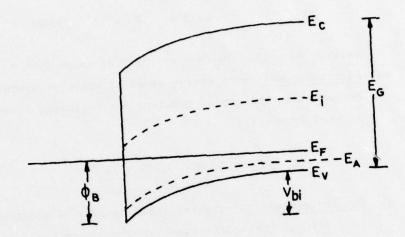


Fig. 4

Energy Band Diagram

For A Schottky Barrier on p-type Silicon

$$E_{q} = 1.165 - 7.242 \times 10^{-3} (T/300) - 3.664 \times 10^{-2} (T/300)^{2}$$
 (1.11)

b) Intrinsic Fermi Level. -- The intrinsic Fermi level E is essentially located at the midgap position, deviating from same in a manner slightly dependent upon temperature, as well as upon the ratio of the effective density of states at the conduction and valence band edges:

$$E_{i} - E_{v} = Eg/2 + (kT/q) ln(N_{v}/N_{c})$$
  
=  $Eg/2 - 1.306 \times 10^{-2} (T/300)$  (1.12)

Here we have used  $(N_{V}/N_{C}) = 1.02/2.8$ , taken from pg. 359 of [12].

c) Acceptor Level. -- The energy level of acceptor states is slightly dependent on the doping density, the following formula being adopted from [13]:

$$E_a - E_v = .0438 - 3.037 \times 10^{-8} N_a^{1/3}$$
 (1.13)

d) <u>Intrinsic Density.</u>—The intrinsic density of electrons and holes is a strongly dependent function of temperature [14]:

$$n_i = 3.925 \times 10^{19} \left(\frac{T}{300}\right)^{3/2} \exp \left\{-qE_g/2kT\right\}.$$
 (1.14)

Here the leading numerical constant has been chosen so as to cause n, to equal 1.5 x  $10^{10}$  cm<sup>-3</sup> when T =  $300^{\circ}$ K.

e) Bulk Hole Density. -- The hole density within the charge-neutral substrate region is related to the intrinsic density and to the Fermi energies  $\mathbf{E}_i$  and  $\mathbf{E}_f$  by the well-known relationship:

$$p = n_i \exp \left\{ q(E_i - E_f) kT \right\}$$
 (1.15)

This, too, is strongly dependent upon temperature.

f) Ionized Acceptor Density. -- The ionized acceptor density is moderately dependent upon temperature, the following being adopted from [13]:

$$N_{a} = \left[\frac{N_{a}}{1 + \left\{4 + 2 \exp\left(\frac{-q\Delta}{kT}\right)\right\} \exp\left\{q \left(E_{a} - E_{f}\right)/kT\right\}}\right]$$
(1.16)

where  $\Delta$  = .044 eV, and accounts for the spin orbit splitting at the valence band maximum in silicon.

The crux of the temperature dependence of the equilibrium parameters is seated in (1.14) through (1.16), with the latter two of these equations involving the extrinsic Fermi level  $E_{\rm f}$ , which is unknown a-priori. That level must self-adjust to satisfy the requirement of charge neutrality in the bulk substrate region. Given the operating temperature T, self-consistent solutions of (1.14) through (1.16) are required which satisfy the condition:

$$N_a + p = 0$$
 (1.17)

(Here, we ignore the small additional charge due to the presence of minority electrons, which constitutes a negligible correction.)

The subprogram of the computer model which treats the determination of the above equilibrium parameters, given the doping density  $N_a$  and the operating temperature T as input data, determines this self-consistent solution of (1.14) through (1.16), using iterative methods.

TABLE I illustrates the temperature dependence of the intrinsic density  $\mathbf{n}_i$ , the ionized acceptor density  $\mathbf{N}_a$ , and the "built-in" potential difference  $\mathbf{V}_{bi}$ , for the case where the acceptor density  $\mathbf{N}_a$  is  $10^{15}$ , and the Schottky barrier height  $\boldsymbol{\varphi}_B$  is 0.27 eV (typical of a platinum-silicide on p-type silicon structure).

т ( <sup>0</sup> к)	n <sub>i</sub> (cm <sup>-3</sup> )	$N_a(cm^{-3})$	V <sub>bi</sub> (Volts)
50	6.73×10 <sup>-41</sup>	1.62×10 <sup>14</sup>	2.30×10 <sup>-1</sup>
100	4.61×10 <sup>-11</sup>	9.16x10 <sup>14</sup>	1.97x10 <sup>-1</sup>
150	6.08×10 <sup>-1</sup>	9.89×10 <sup>14</sup>	1.53x10 <sup>-1</sup>
200	8.08×104	9.97×10 <sup>14</sup>	1.07×10 <sup>-1</sup>
250	1.08×10 <sup>8</sup>	9.98×10 <sup>14</sup>	5.89x10 <sup>-2</sup>
300	1.50×10 <sup>10</sup>	9.99×10 <sup>14</sup>	9.60x10 <sup>-3</sup>
350	5.32×10 <sup>11</sup>	9.99×10 <sup>14</sup>	-4.08×10 <sup>-2</sup>

TABLE I -- Temperature Dependence of the Intrinsic Density  $n_i$ , the Ionized Acceptor Density  $N_a$ , and the Built-in Potential  $V_{\rm bi}$  for a Schottky Barrier on p-type Silicon, for the Case  $\phi_{\rm B}$  = 0.27 ev,  $N_{\rm A}$  = 10<sup>15</sup> cm<sup>-3</sup>

Examining this table, one notes the negligible density of minority carriers (n  $\approx$   $n_i^2/N_a$ ) in comparison with majority carriers (p  $\approx$   $N_a$ ) over the entire temperature range. One also notes the rapid decrease of the "built-in" potential  $V_{\rm bi}$  as the temperature increases. The barrier becomes essentially "ohmic" at temperatures well below  $300^{\rm O}{\rm K}$ . One notes, also, the gradual "freeze-out" of ionized acceptors as the temperature decreases.

The discussion above has been directed toward p-type Schottky barriers. Minor modifications make it applicable to n-type structures as well:

a) One substitutes the n-type barrier height in place of the  $\phi_{\rm B}$  for p-type material. (The sum  $\phi_{\rm Bp}$  +  $\phi_{\rm Bn}$  equals the energy gap  ${\rm E_g}$ ). One also substitutes N<sub>d</sub> in place of N<sub>a</sub>, and interchanges subscripts p and n.

b) One substitutes the ionized donor density  $N_{\rm d}$  in lieu of the ionized acceptor density  $N_{\rm a}$ . The temperature dependence of the former differs from that of the latter (eq. (1.16)), becoming:

$$N_{d} = \left\{ \frac{N_{d}}{1 + 2 \exp \left\{ q(E_{f} - E_{d})/kT \right\}} \right\}$$
 (1.18)

Equation (1.18) differs from (1.16) on two counts: 1) There is no spinorbit splitting in the conduction band; 2) The ground state degeneracy factor for the conduction band is 2, instead of 4.

### CHAPTER II

### Calculations of the Reverse Voltage Breakdown Characteristics of Metal-Silicide Schottky Barriers on P-Type Silicon

In this chapter we present results obtained with the computer model for p-type structures, assuming  $r_{m}$ ,  $\phi_{B}$ ,  $N_{a}$ ,  $Q_{ss}$ , and T are the given parameters.

### 1.0 The Effect of Barrier Radius of Curvature

Figure 5 illustrates the effect of barrier radius of curvature ( $r_m$  in Fig. 1) upon the multiplication ratio M. This figure shows M versus V, using both (1.07) and (1.10) for two-carrier and single carrier multiplication, respectively. These calculations were based upon an assumed N<sub>a</sub> of 1.6 x 10<sup>15</sup> (10 ohm-cm material), and  $\phi_B = 0.27$  ev (simulating a platinum-silicide barrier), at T =  $77^{\circ}$ K. Circular symmetry was used in this calculation ( $x_m = y_m = r_m$ ).

Figure 5 shows that breakdown occurs at progressively lower voltages, with a reduction in radius of curvature. Further, this sequence of calculations show that single carrier multiplication is "softer" in appearance than a two-carrier multiplication process, where  $M=\infty$  at finite reverse voltages.

Figure 5 reveals an interesting trend, however. The smaller the radius of curvature, the more nearly do the curves for two-carrier and single-carrier multiplication coincide at low voltages and currents. Specifically, a two-carrier multiplication process becomes "soft" with a reduction in radius of curvature. The foregoing observation is further illustrated in Figure 6, which is a "blown-up" view of the  $r_m = .01~\mu$  m, curve from Fig. 5.

From Fig. 6, it is suggested that a very shallow platinum-silicide layer could produce a very small radius of curvature and, hence, soft breakdown characteristics at small values of applied biasing voltage.



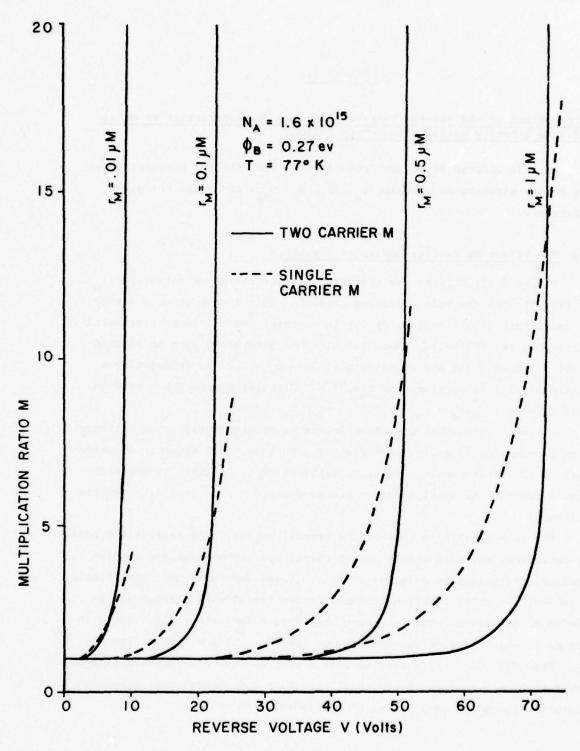


Fig. 5
Multiplication Ratio vs. Reverse Applied Voltage for a Range of Junction Radius of Curvature

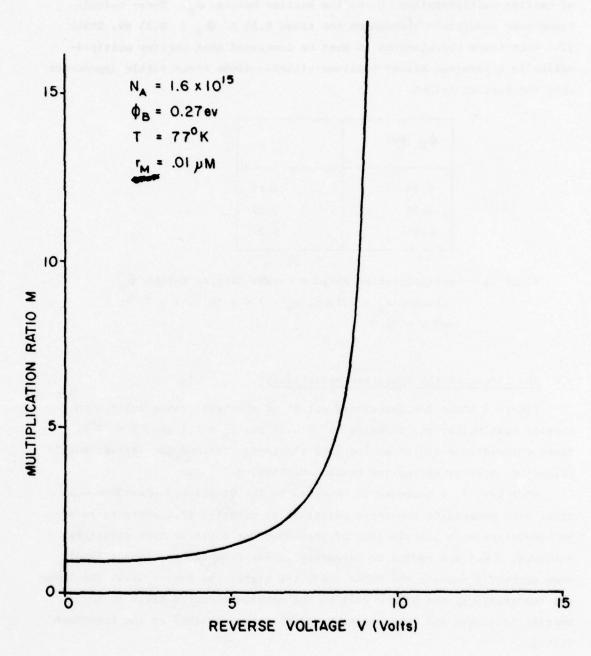


Fig. 6 Multiplication Ratio M vs. Applied Reverse Voltage, Assuming the Radius of Curvature is 100 %

### 2.0 The Effect of the Barrier Height

Breakdown calculations were undertaken to ascertain the sensitivity of carrier multiplication, M, on the barrier height  $\phi_{\rm B}$ . These calculations were undertaken throughout the range  $0.25 \le \phi_{\rm B} \le 0.35$  ev, TABLE II. From these calculations it must be concluded that carrier multiplication in a reversed biased platinum-silicide diode shows little dependence upon the barrier height.

φ <sub>B</sub> (ev)	М	
0.25	5.80	
0.30	6.07	
0.35	6.37	

Table II -- Multiplication Ratio M versus Barrier Height  $\phi_B$  assuming  $r_m = 0.1 \, \mu m$ ,  $N_a = 1.6 \times 10^{15}$ ,  $T = 77^{\circ} K$ , and  $V = 22 \, V$ .

### 3.0 The Effect of the Substrate Resistivity

Figure 7 shows the calculated effect of substrate resistivity upon carrier multiplication, assuming  $\phi_B = 0.27$  ev,  $r_m = 0.1$   $\mu$ m,  $T = 77^{O}$ K. These calculations are shown for both single-carrier and two-carrier multiplication, against an applied biasing voltage, V.

From Fig. 7, a decrease is observed in the calculated breakdown voltage, with decreasing substrate resistivity; clearly, this characteristic is consistent with calculations of breakdown for a planar type structure. Although, a 0.1  $\mu$ m radius of curvature is far from planar, planar theory does correctly predict the trend that, the higher the doping (i.e. the lower the resistivity), the higher will be the maximum electric field at the barrier interface and, therefore, a reduction is obtained in the breakdown voltage.

### 4.0 The Effect of Surface Charge at the Silicon-Silicon Dioxide Interface

The effective surface charge  $Q_{SS}$  is known to arise when  $SiO_2$  is grown on the surface of silicon; this charge is known to be positive, and with

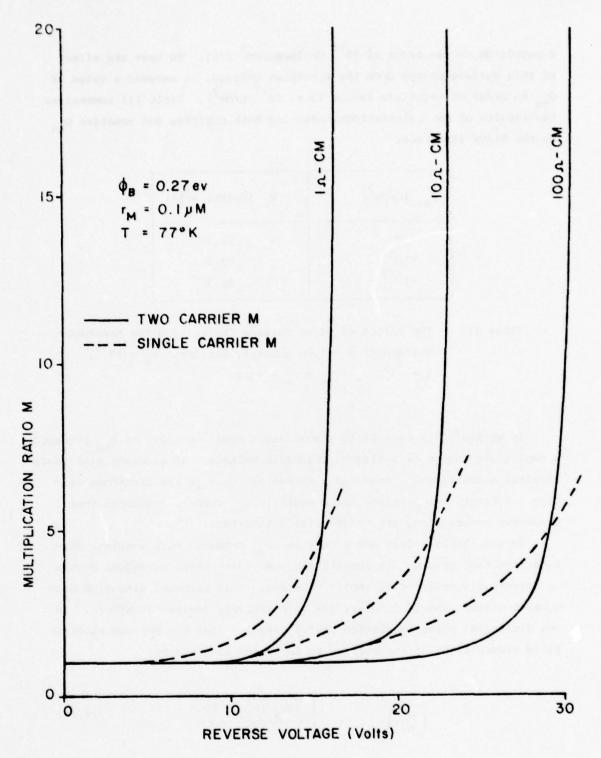


Fig. 7
Multiplication Ratio vs. Applied Reverse Voltage for a Range of Substrate Resistivities,  $r_{\rm m} = 0.1~{\rm um}$ 

a magnitude on the order of  $10^{-8}$  Coulombs/cm<sup>2</sup> [16]. To test the effect of this surface charge upon the breakdown voltage, we assumed a value of  $Q_{SS}$  an order of magnitude larger (i.e.  $10^{-7}$  C/cm<sup>2</sup>). Table III summarizes the results of our calculations, assuming both positive and negative  $Q_{SS}$  at the Si/Ox interface.

Q <sub>ss</sub> (C/cm <sup>2</sup> )	V <sub>b</sub> (Volts) (-5%)
0	52.2
+10 <sup>-7</sup>	49.8
-10 <sup>-7</sup>	32.3

Table III -- The Effect of Oxide Surface Charge upon the Breakdown Voltage of a P-type Schottky Barrier.  $N_a = 10^{16}$ ,  $T = 77^{\circ}$ ,  $x_m = y_m = r_m = 1 \,\mu\text{m}$ .

In general, all calculations assuming a positive value of  $Q_{SS}$  produced a negligible change of avalanche breakdown voltage. In contrast with these results, a negative  $Q_{SS}$  produced a marked decrease in the breakdown voltage. Further, calculations for a negative  $Q_{SS}$  clearly indicated that breakdown occurs along the oxide-silicon interface.

To gain insight into why a negative  $Q_{SS}$  produced such results, consider the case when  $Q_{SS}$  is absent, and the region where breakdown occurs is essentially depleted of mobile carriers. This proposed situation produces a uniform charge density, due to negatively ionized acceptors. In one dimension, planar depletion theory predicts that the maximum electric field occurs right at the barrier surface, and is given by:

$$\left(\frac{d\psi}{dx}\right)_{\text{max}} = \sqrt{\frac{2qN_a (V_{\text{bi}} + V)}{\epsilon}}$$
(1.18)

Note that the higher the negative charge  $N_a$ , the higher the electric field, and therefore the lower the expected breakdown voltage.

Although the planar solution cited cannot predict quantitatively the effect of a surface charge  $Q_{\rm SS}$ , it does predict qualitatively the effect observed in Table III. Locally, a negative  $Q_{\rm SS}$  would augment the negative charge, due to background acceptors, and a local increase in electric field along the surface. Thereby, from a qualitative point of view, it is suggested that a decrease of breakdown voltage will be observed in the vicinity of a negative surface charge. Conversely, a positive  $Q_{\rm SS}$  would tend, locally, to compensate the negative background charge and, thereby, lead to a decrease in electric field, and an associated increase of breakdown voltage. This is generally consistent with our observations in the computer model. Assuming  $Q_{\rm SS}$  positive, breakdown was found to occur well away from the  ${\rm SiO}_2$ -Si interface. Conversely, with  $Q_{\rm SS}$  negative, it occurred right at that interface.

From the foregoing calculations it is suggested that an oxide surface charge  $\mathbb{Q}_{SS}$  (which is physically positive) will have a marked effect on the avalanche breakdown voltage of n-type Schottky barriers, and a negligible effect upon p-type structures.

# 5.0 The Effect of Temperature

Figure 8 presents the calculated breakdown voltage for two-carrier multiplication, as a function of temperature T, for the case N = 1.6 x  $10^{15}$ ,  $\phi_{\rm B}$  = 0.27 eV, and r = 0.1  $\mu$  m. As previously stated, the computer model utilizes Crowell and Sze's empirical fit to Baraff's curves to estimate the Townsend ionization coefficients  $\alpha_{\rm B}$  and  $\alpha_{\rm C}$  at reduced temperatures. We find that this empirical fit does not adequately agree with published experimental data at temperatures well below  $300^{\circ}$  K. For this reason, there remains many questions as to whether the specific shape of the curve in Figure 8 is more than qualitatively correct.

From Table I, however, it is clear that a p-type platinum-silicide Schottky barrier goes ohmic at temperatures approaching room temperature. This situation implies that large reverse currents will be observed at voltages well below the  $\approx$  22 volt value shown in Figure 8. For this reason, it appears physically meaningless to undertake breakdown calculations at temperatures such that the "built-in" potential  $V_{\rm bi}$  is on the order of a few (kT/q), or less. Mechanisms other than avalanche breakdown come into play at elevated temperatures, and these mechanisms produce

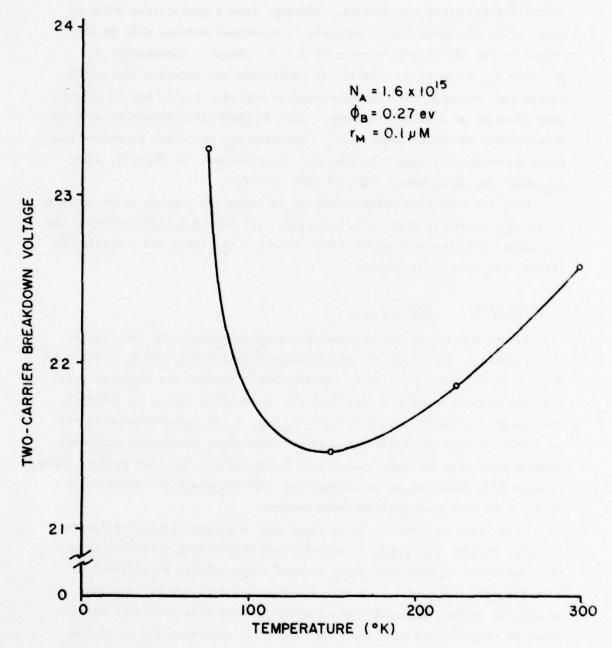


Fig. 8
Calculated Breakdown Voltage for a Two-Carrier
Multiplication Process vs. Junction Temperature

large reverse currents at reverse voltages well below those required for significant carrier multiplication.

#### CHAPTER III

#### Instructions for Using the Computer Program

## 1.0 Input Data

Input data are specified in the form of NAMELIST data sets: GEOM, PRMTRS, CONTRL, SWITCH, and SINGLE. Table IV shows a sample set of such input data.

AGEOM XWIDTH=0.10, YDEPTH=0.10, IMAX=31, JMAX=31, NXMDTH=17, NYDPTH=17, XDELTA=1.00, YDELTA=1.00, RAD=0.10, GEND

@PRMTRS ACCPTR=1.6E15, BRRIER=0.27, QSS=0.00E-09, TMPTR=077.0, GEND

@CONTRL ITMAX=25, ITRMAX=25, CONVRG=0.02, SIDLT=0.005, AVDLT=.01, VLTDLT=.05, KNTMAX=100, GEND

@SINGLE VOLTO=5.0, DLTVLT=5.0, NVOLT=5, KOUTPT=1, GEND

@SWITCH NDOPE=0, GEND

SCHOTTKY BARRIER--SOFT BREAKDOWN CASE

QSS=0.E-00 RAD=.10

Table IV -- Sample Input Data

Note that the last 3 cards of the data set are for a 3-line title; thereby a user may identify the purpose of any particular run. It is emphasized that these 3 title cards must be present in the data deck, even if they are left blank. Immediately following the input of these data, the title is printed, in addition to a listing of all input data.

As discussed in Chapter I, two versions of the program exist, the first version iterates the applied voltage to ascertain the applied voltage leading to breakdown, the second version increments the applied voltage over a specified range, and at specified increments. The latter are specified in NAMELIST/SINGLE/. In the event that the first version of the program is being used, NAMELIST/SINGLE/ should be omitted. Failure to do so will result in an EXIT.



It is also emphasized that the order in which these NAMELISTS appear in the data deck must be retained.

# 1.01 NAMELIST/GEOM/

This data set specifies the geometry to be treated, and it includes:

XWIDTH -- Width of the metal-silicide region in microns (x of Figure 1).

YDEPTH -- Depth of the metal-silicide region in microns ( $y_m$  of Figure 1).

IMAX -- Total number of lattice points in the x-direction of Figure 1 (31 maximum).

JMAX -- Total number of lattice points in the y-direction of Figure 1 (31 maximum).

NXWDTH -- Number of lattice points in the x-direction which overlay the metal-silicide region (a fraction of IMAX).

NYDPTH -- Number of lattice points in the y-direction which overlay the metal-silicide region (a fraction of JMAX).

XDELTA -- The parameter  $\delta$  ( $\leq$ 1) described below.

YDELTA -- The parameter  $\delta_{_{_{\mathbf{V}}}}$  (  $\leq$  1) described below.

RAD -- Radius of curvature of the metal-silicide corner, in microns (r<sub>m</sub> of Figure 1).

The parameters  $\delta_{\chi}$  and  $\delta_{\gamma}$ , represented by XDELTA and YDELTA above, control the grading of the lattice illustrated in Figure 2. Both XDELTA and YDELTA must be assigned numerical values  $\leq$  1. (In generating the graded lattice of Figure 2, XDELTA and YDELTA were equal, with a magnitude of 0.85). These grading parameters function in the following manner.

Let  $\Delta x$  be the interval between two horizontal lattice points located at I and I-1 (where  $2 \le I \le NXWDTH-1$ ). The interval  $\Delta x'$  between the lattice points located at I and I + 1 is given by the algorithm  $\Delta x$  (I + 1) =  $\delta_x \Delta x(I)$ . Thus, with  $\delta_x < I$ , the spacing between adjacent lattice points gradually reduces to smaller and smaller values as the index I increments from 2 to NXWDTH-1. The parameter  $\delta_y$  plays a similar role in grading the vertical lattice spacings within the rectangle which overlays the metal-silicide region. Note that setting both  $\delta_x$  and  $\delta_y$  equal to unity leads to a uniform lattice spacing in that region, which is really

the best choice when the geometry treated has circular symmetry (i.e.  $x_m = y_m = r_m$  in Figure 1).

It will be noted that the parameters XDELTA and YDELTA are used only for the rectangle which overlays the metal-silicide region. The grading of the remaining lattice spacings (for NXWDTH < I < IMAX and NYDPTH < J < JMAX) is achieved automatically, once the lattice for the metal-silicide region has been determined. Multipliers analogous to XDELTA and YDELTA are determined in order to apportion the remaining lattice points throughout a distance of 1.25 depletion widths, as shown.

### 1.02 NAMELIST/PRMTRS/

ACCPTR -- The acceptor density  $N_a$  (cm<sup>-3</sup>). (To treat n-type material, this parameter must be assigned the numerical value of the donor density.)

BRRIER -- The Schottky barrier height  $\phi_{_{
m R}}$  (ev).

QSS -- The oxide interface interface charge  $Q_{gg}$  (C/cm<sup>2</sup>).

TMPTR -- The operating temperature T (OK).

# 1.03 NAMELIST/CONTRL/

This data set specifies parameters which control the iterative procedures used within the computer model.

- ITMAX -- Maximum number of iterations to be allowed in the implementation of Gummel's algorithm. The program will stop execution, and a termination message will be printed if ITMAX is exceeded.
- ITRMAX -- Maximum number of iterations to be allowed in the implementation of Stone's method. The program will stop execution, and a termination message will be printed if ITRMAX is exceeded.
- CONVRG -- Convergence criterion for Gummel's algorithm.

MAX 
$$|\psi_m - \psi_{m+1}|$$
 < CONVRG, where m is the iteration number

- SIDLT -- Convergence criterion for Stone's method. When the maximum of the absolute residual (see Stone's paper for its definition) is found less than SIDLT, Stone's method is taken to have converged.
- AVDLT -- Convergence criterion for the method of secants in SUBROUTINE AVLNCH. When the denominator in eq. (1.07) is found to have an absolute value less than AVDLT, convergence is satisfied.

- VLTDLT -- Convergence criterion for the outer iterative procedure used in SUBROUTINE AVLNCH. When the new value of V is within VLTDLT x 100% of the previous value, convergence is satisfied.
- KNTMAX -- Maximum number of points allowed per trajectory in SUBROUTINE AVLNCH. If this is exceeded, execution will stop, and a termination message will be printed, explaining any necessary corrective action.

The sample input data contained in Table IV give values for the above parameters which have been found to work satisfactorily.

### 1.04 NAMELIST/SINGLE/

This data set is required only when the second version of the program is used. These parameters are designed to step the applied voltage through a prescribed range, listing M (the carrier multiplication) for both two-carrier and single-carrier processes. This data set should be omitted if the first version of this program is to be used.

- VOLT  $\phi$  -- The initial (lowest) voltage to be used (volts).
- DLTVLT -- The voltage increment (volts) for stepping the applied voltage upwards.
- NVOLT -- The number of applied voltage values to be treated.
- KOUTPT -- A switching parameter used to bypass the printing of voluminous output of two-dimensional tables. Set KOUTPT =  $\phi$  if detailed data printout is desired. Set KOUTPT = 1 if these data are not required.

#### 1.05 NAMELIST/SWITCH/

This data "set" contains a single parameter used to flag whether p-type or n-type material is to be treated.

NDOPE -- Set NDOPE =  $\phi$  if the substrate is to be considered p-type, or NDOPE = 1 if the substrate is n-type.

#### 2.0 Output Data

The output data printed with the computer model will first be discussed in the context of the second version of the computer program, wherein the

applied reverse voltage is incremented in pre-specified steps. Alterations of the data format for the other version will then be discussed separately.

# 2.01 Output Data for the Version Which Increments the Applied Voltage in Prespecified Steps

Table V (2 sheets) illustrates the output obtained with the former version. Note that the title that was included with the input data is first printed, followed by a summary of the data specified in the five input NAMELIST sets. This is followed by a summary of the equilibrium parameters at the specified temperature T (77°K in this case). These data are:

TMPTR -- The temperature (OK)

EGAP -- The energy gap Eg (ev)

EIV -- The energy difference (E; - E) of Figure 4

EFV -- The energy difference  $(E_f - E_V)$  of Figure 4

TRNSIC -- The intrinsic carrier density  $n_i$  (cm<sup>-3</sup>) at temperature T.

BKGRND -- The background density of ionized impurities (cm<sup>-3</sup>) at that temperature

VBLTIN -- The "built-in" potential (volts) of Figure 4

Following the above listing, information is given allowing one to follow the progress of the iterative procedure. The case illustrated possesses circular symmetry  $(x_m = y_m = r_m)$  and therefore the initial guess for  $\psi$  obtained from cylindrical coordinate depletion theory is a reasonable approximation. In this example three iterations of Stone's method were required, and a single application of Gummel's algorithm was sufficient to achieve convergence.

Subsequent to this convergence of the iterative procedure for each voltage step the following data are tabulated:

K -- K = 2 signifies that the central trajectory of the triplet of trajectories normally investigated is the one for which the data are listed. (Actually, because of the circular symmetry of the case illustrated, it was the only one treated.) SCHOTTAY BANKIEM-SUIFT INEAKOURN CASE USSENEE-NO MADE 10 A.U. SUINEMERNÖ 10/51/78

ut Input DAFA : SUMMARY

MARTELIST/DEDMY XMIDTHS 1.075-01 TREPTHS 1.00E-01 IMAKS 51 MAKS 51 MKMUTHR 17 NYUPTHR 11 KDELTAS 1.00E+00 THP THE 7.70E+01 PAULIS 1.30E-02 VLTDLIR 5.00E-02 KINLIS 1.30E-03 MARELISTYMHTHS/ ACCPTUR 1. ANE . 15 HAMIEME 2.70E-01 4358 0.0

MATTELIST/31MGLE/ VULTOR S.NOE+NO DLTVLIR S.UNE+00 MVILIR S KUUTPIR 1

MAMELISIZAMITCHZ NUMPER O

7.70£+01 1.10£+00 5.77£-01 5.24£-01 5.34k-02 5.44k-20 1.02f+15 2.17k-01 BRGHND THNSIC EF. EGAP

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Sample Output Data (Vapp stepped)

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ISTANT	2	VALTA 3 17EP NAX DE	181441	2 2 3 - 3	2
*	~		* • •		۸ .

I START -- The indices (I, J) of the lattice point at the upper left corner J START of the "box" containing the starting location of the trajectory.

XPATH -- The (x, y) coordinates (in microns) of the charge trajectory as
YPATH time of flight increases.

ET -- The total electric field  $(E_t = \sqrt{E_x^2 + E_y^2})$  (in V/cm) at that location.

ALPHN -- The Townsend coefficients  $\alpha_p$ ,  $\alpha_p$ , obtained from Crowell and ALPHP Sze's empirical fit to Baraff's curves (cm<sup>-1</sup>).

PI -- The value of the integral in eq. (1.10) for the care of single-carrier multiplication.

OMEGA -- The value of the integral in eq. (1.07) for the care of twocarrier multiplication.

Note that the two integrals converge to a constant value as the charge trajectory extends into regions of small electric field. The numerical integration terminates when the most recent value for  $\Omega$  is within .01% of its previous value.

Following the above tabulations are printed the parameters:

VOLT -- The applied voltage V (volts)

M1 -- The single-carrier multiplication ratio given by eq. (1.10).

M2 -- The two-carrier multiplication ratio given by eq. (1.07).

For the case illustrated, note that the latter changes sign (because the integral  $\Omega$  exceeds unity) with V=25 volts. This signifies that avalanche breakdown occurred at a voltage somewhere between 20 and 25 volts, for this case. (Figure 5 shows it to occur at V=22.6 volts.)

The case illustrated in Table V was run with KOUTPUT = 1, thereby bypassing the printing of additional output data. Had KOUTPT = 0, however, additional tables of data showing would have been listed. These tables are all formatted in an identical manner, so it suffices to illustrate and discuss only one of them.

Table VI (2 sheets) illustrates the data listed for the electrostatic potential, in unnormalized units. These data were generated for a case differing from the one discussed above. One reads the table in the following manner. Listed across the top of the first sheet are the x-coordinates X(I) of the lattice, in microns. Just below that are the headings  $^*J$ , Y(J),

		# (1), Tel, TH	*								
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9	1.00E.02	24.00 94.00 94.00 94.00 11.00	8.81E+01	2.49E-01	22.4 20.4 20.4 20.4 20.4 20.4 20.4 20.4	2.046.01 3.156.001	1.92E+01	3.75 E	2.60 80 80 80 80 80 80 80 80 80 80 80 80 80	2.04.0 2.04.0 6.001	1.275.00
2	2.00E-02	4400 ### ###	8.39E 8.18.001	2.49E.01	24 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	2.04. 3.04. 3.04. 3.01. 3.01. 3.01.	2.00 1.92 1.92 1.01 1.01	3.746	2.00 8.00 8.00 8.00 8.00 8.00 8.00 8.00	04.6 04.6 04.6 04.6 04.6 04.6 04.6 04.6	10000000
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<b>~</b>	4.00E-02	2.44 2.44 6.04 6.04 6.04 6.04 6.04	2.49E.01	2.49E+01	2.46E+01	3.00 3.15E.001	1.909 1.905 1.905 1.905	3.7.8 6.7.5 6.01	2.54 8.54 8.00 8.00 8.00 8.00	2.47E-01	2.049E-01
2	5,01E-02	0.30 0.30 0.00 0.00 0.00 0.00 0.00	2.44E+01	2.24E-01	2.14E+01	2.075.01 3.15E.00	1.00 9E	3.74E+01	2.5 8.5 8.5 8.5 8.5 8.5 8.5 8.5 8.5 8.5 8	2.5	2.44E-01
2	A.00E-02	2.35E+01	2.29E-01	6.85E+01	22.12E+01	2.01E.01	11.00 P. 00.1	3.676.01	21.5 22.6 23.6 20.0 20.0	2.44 8-46 001	1.24 E . 01
2	7,006-02	2.32 2.32 2.32 2.32 3.32 3.32 3.32 3.32	2.266.01 6.776.00	2.19E+01 6.85E+01	2.10E+01	3.14E-001	1.07E+01	3-4-4-6-6-6-6-6-6-6-6-6-6-6-6-6-6-6-6-6-	2.57E.01	3.55.00 3.55.00	2.37£-01 0.0
2	9.006-02	2.22.00 0.00.8400 100.8400	2.27E+01	2.49E.01	2.07E+01	3.97E.01	12.00 4.00 4.00 4.00 6.00 6.00 6.00 6.00 6	3.72 6.72 6.01	2.87E-01	1.69E-01	N. 37 E. 001
~	9.00E-02	4400 84500	2.19E-01	8-1-0 8-1-0 8-1-0 1-0 1-0 1-0 1-0	400 400 6 9 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	3.95E.01	1.00 4.00 4.00 4.00 4.00 4.00 4.00 4.00	3.575	2.37E-01	2.33E.01	2.0.1E.01
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2	1.106-01	4100	2.10E-01	2.05E-01	2.37E-01	3.13E.001	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	3.50 3.60 3.60 3.60 3.60 3.60 3.60 3.60 3.6	825	2.59E-01	2
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•	1.405-01	2000 2000 2000 2000	8.54E-01	1.44E-01	8 9 E 001	3.12E.001	11.14	3.56	2.509E-01	2.07E.01	2.046.01
.,	1.436-01	2.046.01	2.048.01	2.048.01	2.058.01	2.048.01	10.300.5	2.01E+01	10.306.1	1.975+01	1.916.01

TABLE IV Electrostatic Potential in Un-normalized Units

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0000	011. 06099 0609 0609	01.27E	000 W W W W W W W W W W W W W W W W W W	03.60E	44W0 44+ 44+ 600	www.o	0.00 0.00 0.00 0.00 0.00	0.00 Bar + 000 B	06.00 06.00	0000 0000 0000	0.225 0.225 0.035	0.00 0.00 0.00 0.00 0.00	0.75 mm + + + + + + + + + + + + + + + + + +	0000	00000 V-V	011
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000	1.91E-03	1.27E-05	23.13E-03	23.71E-01	11. 12. 13. 13. 15. 15. 15. 15. 15. 15. 15. 15. 15. 15	000 000 000	3.84 2.65 2.56 2.56 2.56 2.56 2.56 2.56 2.56	#06 WD0 MMM +++	400 000 000 000	500 525 644 600	5.24E+001	277E	450 200 200	5.65E+001	1.91E+01	6.74E+01
000	01.00	5.47E-05	3.14E-03	2.675-01	440 440 441 441 600 600	134 6000 6000	0000 0000 0000	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	3.75E+00	100	# 100 # 100 # 100 # 100 # 100	4++ +++ 000	### ### ### 000	74501	791	4.825.01
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000	2007E-003	9.75E-05	3.17E-03	0.30	011 035 E • 000	3.13E+00	0.57E-00	040	07.4 AE - 000	0.736.001	0.796.00	004	0-5	1.77E-01	0.1 46.01	1.208.01

and PSI(I, J), I = 1, IMAX, indicating that each subsequent grouping lists the potential along a particular row of the lattice (whose index is J and whose y-coordinate is Y(J), in microns). Thus, first scanning the listing of X(I), one then locates the corresponding potential and the y-coordinate Y(J) in the grouping labeled J. In this manner, the two-dimensional solutions may be determined.

# 2.02 Output Data for the Version Which Iterates the Applied Voltage to Determine Avalanche Breakdown

Table VII (3 sheets) illustrates the output data printed for the alternate version of the computer program. The initial printout, including the equilibrium data, remains the same as that of the previous subsection.

Following that is listed the initial voltage estimate (obtained from SUB-ROUTINE VGUESS) with which the iterative procedure starts. Next follows the summary of the iterative process which, in this case, requires more iterations with both Stone's method and Gummel's algorithm. This is because this version of the program uses planar depletion theory to supply an initial estimate for potential—an estimate which decreases in accuracy, with a decrease in radius of curvature.

With the solution of Poisson's equation now known, the program next deals with triplets of trajectories, labeled K = 1, 2, 3, respectively, as it searches for the trajectory producing the maximum value of the integral appearing in equation (1.07). Normally, the next sequence of data printed would be a multiple set similar to that typified by the single set seen following the iteration summary in Table VII, detailing what is taking place in this search process. For the case illustrated, however, the problem has circular symmetry, and the print-out is unnecessary. Thus, only a single subset of summary data appears in the table, for the trajectory K = 2.

The data included in this subset are:

K -- The label assigned to the trajectory

ISTART -- The starting indices of the trajectory JSTART

XSTART -- The starting coordinates (x, y) of the trajectory, in microns. YSTART

NAMPLIST/GEOM/ XMIDTHS 1.00E-01 YDEPTHS 1.00E-01 IMAXS 31 JMAXS 31 NXWDTHS 11 NYDPTHS 11 XDELTAS 1.00E+00 YNELTAS 1.00E+00

SCHOTTKY BARRIER--SHALLOH-- 77 DEG K 0.59mn A.D. SUTHERLAND--4, 20, 78

THPTR. 7.70Eval

NAMELIST/CONTAL/ ITMAKE 24 ITRMAME 24 CONVRGE 2.00E-02 SINLTE 5.00E-03 AVDLTE 1.00E-02 VLIDLTE 5.00F-02 KNTMAKE 100

NAMELIST/PRHTRS/ ACCPTRe 1. BAE-15 BPHTERE 2,70E-01 0550 0.0

SUMMARY OF INPUT DATE :

7.70E+n1 1.16E+00 5.77E+n1 9.24F+n1 5.32E+n2 5.24E+20 1.02E+15 2.17E-n1

VBLTIN

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FGAP

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TABLE VII Sample Output Data (Avalanche Calculation)

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9 ITERATIONS WERE REDUTRED IN GRFLAX

10

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	2 1	2 4	S	. 1

PRESIDE NI CONTRA PROJECT MITH STONE - METHOD IN POSSES &

MAX DELTA IN GRELAX IS 3.673E-D2 AT COORDINATE ( 1, 6)
S ITERATIONS MERE REQUIRED MITH STONES METHOD IN POISSN
MAX DELTA IN GRELAX IS 2.399E-D2 AT COORDINATE (25, 7)
A ITERATIONS WERE REQUIRED MITH STONES METHOD IN POISSN
MAX DELTA IN GRELAX IS 2.047E-D2 AT COORDINATE (26,31)
A ITERATIONS WERE REQUIRED MITH STONES METHOD IN POISSN
MAX DELTA IN GRELAX IS -1.516E-D2 AT COORDINATE ( 1,13)
9 ITERATIONS WERE REQUIRED IN GRELAX

XPATH -- The coordinates (x, y), in microns, of the moving charge as time YPATH progresses.

ET -- The total electric field  $E_{+}$  (V/cm) at that location

ALPHA -- The Kennedy-O'Brien value for  $\alpha$  .

PI -- The value of the integral in the denominator of (1.07)

With the trajectory maximizing PI determined, the program next modifies the applied voltage iteratively, scaling E<sub>t</sub> along the trajectory in the manner described in Chapter I, and respects the evaluation of the integral PI until the most recent two values bracket unity. Again, subsets of summary data are printed during this search for the bracketing condition, so that the process can be monitored. In the case illustrated, this bracketing required only a single step, so only a single subset of such data were printed. Normally, more than one such subset might be expected to appear.

This subset lists the following parameters:

KEY -- a flag; when equal unity indicating iteration subset

PSINRM-- The total voltage  $(V_{hi} + V)$  in volts

DSTNRM-- The (planar) depletion width W<sub>d</sub> (cm)

KNT -- A counter for the number of trajectory points in the numerical integration

DX -- Incremental distances (cm) along the path of the numerical in-DY tegration

ET1 -- The electric field E at the beginning and end of the integration interval

ALPHA -- The Kennedy-O'Brien empirical Townsend coefficient  $\alpha$ 

PI -- The ionization integral in the denominator of eq. (1.07) with  $lpha_{_{
m D}}$  and  $lpha_{_{
m D}}$  replaced by lpha

Upon finding two adjacent trial voltages which cause the ionization integral PI to bracket unity, the secants technique is used to zero in on the voltage which causes PI to equal unity. The flag KEY is set to 2 for this next sequence of steps. Again, a number of subsets of data are

printed, each time the root-finding program goes through one of its iterations. In the case illustrated, only one such subset was printed because the program converged to the desired voltage in a single iteration. The parameters in this subset are the same as those just defined above.

The above data have all been determined using the first solution of Poisson's equation for the initial estimate of the applied voltage V. Now that a revised estimate for this voltage is available an updated solution of Poisson's equation is obtained, and the process is repeated. Again, a summary of the convergence of the iterative determination of the solution of Poisson's equation is listed, etc. In the case illustrated, the revised estimate of the applied voltage required for breakdown was within the 5% convergence range specified by VLTDLT in NAMELIST/CONTRL/, and so the execution was terminated.

Rather than a STOP, when convergence of this process is detected, this version of the program first prints all of the two-dimensional data exemplified by Table VI (not repeated in Table VII), then prints the resultant breakdown voltage. Then the program loops back to the beginning and searches for a complete new set of input data. This allows multiple cases to be treated in one run. Failing to find such additional data, the program exits.

# CHAPTER IV

#### Conclusions

Several different mechanisms could produce enhanced reverse current (or breakdown) in a Pt-Si Schottky barrier diode. In two spatial dimensions, a small radius of curvature at the junction periphery would locally increase the space-charge layer electric field and, hence, increase carrier multiplication. The existence of surface states at the metal-Si interface (and an associated  $Q_{_{SS}}$ ) could also enhance the reverse current (or breakdown), although this mechanism should not be significant in p-type devices. Similarly, lattice strain, micro-cracks, or other lattice damage could produce an enhanced reverse current; the presence of these lattice defects appear unlikely to produce a true breakdown situation.

Clearly, there are several potential explanations for the large reverse current exhibited by p-type Pt-Si barriers. Our initial direction was to attribute this reverse current to a classical Townsend avalanche process, and to model this process in two spatial dimensions. After the computer model became operational, substantial qualitative differences were observed between the reverse volt-ampere characteristics of a laboratory device and calculated results. Most laboratory devices exhibit a relatively soft reverse characteristic, whereas the computer model predicted a relatively abrupt reverse breakdown. This comparison between experiment and theory suggested that the reverse current of laboratory devices could be attributable to mechanisms other than avalanche breakdown.

From Townsend's theory of carrier multiplication it is known that one-carrier processes yield a relatively soft breakdown characteristic. Further, other workers have suggested that the ionization rate of electrons at low temperatures is substantially greater than the ionization rate for holes. It is for this reason that a one-carrier multiplication process becomes a possible mechanism to explain the reverse volt-ampere characteristics of these devices. An important question arises concerning the available density of electrons in p-type silicon at  $70^{\circ}$ K. Calculations for ideal p-type material indicate an electron density (at  $70^{\circ}$ K) that is too low to produce a significant amount of reverse current.

It is suggested that lattice strain between Pt/Pt-Si/Si is sufficient to produce substantial lattice damage, and a ready source of free electrons. Such lattice damage has been reported in the technical literature. Further, it is suggested that lattice damage arising in devices containing a large quantity of Pt is an important reason why they are of poor electrical quality. Most workers find it necessary to use very small quantities of Pt to successfully fabricate a Pt-Si Schottky barrier.

Assuming lattice damage produces the necessary electrons, a one-carrier multiplication process could explain the soft reverse current characteristics observed in laboratory experiments. Further, theory predicts that one-carrier multiplication processes yield an exponential increase of reverse current, with an increase of reverse voltage. Crude evaluations of practical devices show that an exponential volt-ampere relation is frequently observed over a substantial range of reverse bias. For this reason, one-carrier multiplication could provide a substantial portion of the excessive reverse current in p-type Pt-Si Schottky barrier diodes.

In conjunction with studies unrelated to this effort it was realized that other mechanisms could produce an exponential reverse volt-ampere characteristic. In particular, carrier tunneling at the metal-Si interface could yield an exponential volt-ampere characteristic, similar to that predicted for one-carrier multiplication. A very crude model was developed for tunneling at the Pt-Si interface; this model qualitatively established the suspected volt-ampere relation, although quantitative results were of little value.

From this effort it is concluded that additional work is needed before an adequate model is available for reverse breakdown in a p-type Pt-Si device. At this point reverse current appears attributable to either a one-carrier multiplication or to tunneling at the Pt-Si interface. Before the dominant mechanism becomes identifiable, an accurate quantum mechanical solution should be obtained for tunneling through the Pt-Si interface barrier, as a function of an applied reverse biasing voltage. With such a model, it is suggested that reverse current calculations for a p-type Pt-Si barrier would yield information important to the solution of this fundamental device problem.

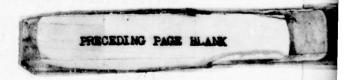
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# Appendix A

Computer Program Listing For Calculating Single and Two-Carrier Multiplication at Specified Voltage Increments

Subroutine	Page
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```
MAIN
C
000
      EXECUTIVE PROGRAM
      INITIALIZE ALL ARRAYS TO ZERO WITH A BLOCK DATA SUBPROGRAM
C
      BLOCK DATA
      COMMON/ARRAYS/ADUMNY(12493), IDUMNY(961)
      COMMON/COEFF/CDUMMY(4931)
      DATA ADUNMY/12493*0./,IDUMMY/961*0/
      DATA CDUMMY/4931*0.E0/
      END
cc
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRHSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/INAX, JMAX, IXNOTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONVRG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
      COMMON/SHGLE/VOLT0, DLTVLT, NVOLT, KOUTPT
      COMMON/SWICH/ NDOPE
C
      DIMENSION TITLE (54)
      DIMENSION XPATH(100,3), YPATH(100,3), ET(100,3)
C
      NAMELIST/GEOM/XUIDTH,YDEPTH,IMAX,JMAX,NXWDTH,NYDPTH,
     &XDELTA, YDELTA, RAD
      NAMELIST/PRMTRS/ACCPTR/BRRIER/QSS/TMPTR
      NAMELIST/CONTRL/ITMAX,ITRMAX,CONURG,SIDLT,AUDLT,ULTDLT,KNTMAX
      NAMELIST/SINGLE/VOLT0, DLTVLT, NVOLT, KOUTPT
      NAMELIST/SWITCH/ NOOPE
  100 READ(5,GEOM)
      READ(5, PRMTRS)
      READ(5, CONTRL)
      READ(5,SINGLE)
      READ(5, SWITCH)
      READ(5,1000) (TITLE(I), I=1,54)
 1000 FORMAT(18A4/18A4/18A4)
      IXWDTH=NXWDTH
      JYDPTH=JMAX-NYDPTH+1
      WRITE(6,1010)(TITLE(I), I=1,54)
 1010 FORMAT(1H1,60%,/,30%,18A4,/,30%,18A4,/,30%,18A4,///5%,'SUMMARY
     &OF INPUT DATA : ',//)
      WRITE(6,1020) XWIDTH, YDEPTH, IMAX, JMAX, NXWDTH, NYDPTH,
     &XDELTA, YDELTA, RAD
 1020 FORMAT(1H0,5%,'NAMELIST/GEOM/ XWIDTH=',1PE10.2,2%,'YDEPTH=',
     &1PE10.2,2X,'IMAX=',I3,2X,'JMAX=',I3,2X,'NXWOTH=',I3,2X,
&'NYOPTH=',I3,2X,'XDELTA=',1PE10.2,/,6X,'YDELTA=',1PE10.2,2X,
     &'RAD=',1PE10.2,/)
```

```
WRITE(6,1030)ACCPTR, BRRIER, QSS, TMPTR

1030 FORMAT(1H0,5%, 'NAMELIST/PRNTRS/ ACCPTR=',1PE10,2,2%, 'BRRIER=',
&1PE10,2,2%, 'USS=',1PE10,2,2%, 'TMPTR=',1PE10,2)
WRITE(6,1040) ITMAX, ITRMAX, CONURG, SIDLT, AUDLT, ULTDLT,
&KNTMAX

1040 FORMAT(1H0,5%, 'NAMELIST/CONTRL/ ITMAX=',13,2%, 'ITRMAX=',
&13,2%, 'CONURG=',1PE10,2,2%, 'SIDLT=',1PE10,2,
&/,6%, 'AUDLT=',1PE10,2,2%, 'ULTDLT=',1PE10,2,2%, 'KNTMAX=',14,/)
WRITE(6,1050) UOLTO, DLTULT, NUOLT, KOUTPT

1050 FORMAT(1H0,5%, 'NAMELIST/SINGLE/ UOLTO=',1PE10,2,2%, 'DLTULT=',
&1PE10,2,2%, 'NUOLT=',12,2%, 'KOUTPT=',12,%)
WRITE(6,1060) NDOPE

1060 FORMAT(1H0,5%, 'NAMELIST/SWITCH/ NDOPE=',12,/)

CALL AULNCH(ULTDLT, AUDLT, XPATH, YPATH, ET, KNTMAX)
GO TO 100
END
```

```
SUBROUTINE GRID
CCCC
      SETS UP THE GRADED LATTICE & COMPUTES THE FINITE-DIFFERENCE
      COEFFICIENTS FOR PSI.
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YOELTA
      COMMON/INTGR/IMAX.JMAX.IXWDTH.JYDPTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/HRNLZE/DHSHRM, PSIMRM, DSTHRM, BLTZMN
      COMMON/RSCALE/ RSFCTR
      FIRST TREAT THE CORNER REGION BOUNDED BY XWIDTH & YDEPTH.
      IMX=IXWDTH-1
      X=XDELTA
      KEY=1
      GO TO 200
  100 XDLT(2)=XWIDTH*DLT
      DO 110 I=3, IXWDTH
  110 XDLT(I)=XDLT(I-1)*XDELTA
      IMX=JMAX-JYDPTH
      X=YDELTA
      KEY=2
      GO TO 200
  120 YDLT(JMAX)=YDEPTH*DLT
      DO 130 J=2,IMX
      JJ=JMAX+1-J
  130 YDLT(JJ)=YDLT(JJ+1)*YDELTA
cccccc
      NEXT TREAT THE REGION EXTERNAL TO THE CORNER REGION. THIS REGION
      EXTENDS 1.25 DEPLETION WIDTHS TO THE RIGHT OF X=XWIDTH; AND
      BELON Y=YDEPTH. USE THE METHOD OF SECANTS TO DETERMINE THE
      MULTIPLIERS ANALOGOUS TO XDELTA & YDELTA LEADING TO A SMOOTH
      TRANSITION IN THE LATTICE SPACINGS AT THE INTERFACE OF THE
      THO REGIONS.
      KEY=3
      KED=1
      CC=XDLT(IXWDTH)/(1.25*RSFCTR)
      X1 = 1.
      IMX=IMAX-IXWDTH
      Y1=(1./IMX-CC)/CC
      GO TO 230
  140 XDLT(IMAX)=1.25*RSFCTR*DLT
      DO 150 I=2, INX
      II = IMAX + 1 - I
  150 XDLT(II)=XDLT(II+1)*X
      KED=2
      CC=YDLT(JYDPTH+1)/(1.25*RSFCTR)
      X1 = 1.
```

```
INX=JYDPTH-1
      Y1 = (1. \angle IMX - CC) \angle CC
      GO TO 230
  160 YDLT(2)=1.25*RSFCTR*DLT
      00 170 J=3.JYDPTH
  170 YOLT(J)=YOLT(J-1)*X
      XDLT(1)=XDLT(2)
      XDLT(IMAX+1)=XDLT(IMAX)
      YDLT(1)=YDLT(2)
      YDLT(JMAX+1)=YDLT(JMAX)
CCC
      FINITE-DIFFERENCE COEFFICIENTS
      DO 175 I=1, IMAX
      DO 175 J=1, JMAX
      XAU=(XDLT(I)+XDLT(I+1))/2.
      YAU=(YDLT(J)+YDLT(J+1))/2.
      QAREA(I,J)=XAU*YAU
      HSTH(I,J)=XAU/YDLT(J)
      HNEST(I,J)=YAU/XDLT(I)
      HEAST(I,J)=YAU/XDLT(I+1)
      HNRTH(I,J)=XAU/YDLT(J+1)
  175 HCNTR(I,J)=-(HSTH(I,J)+HWEST(I,J)+HEAST(I,J)+HNRTH(I,J))
CC
      TABULATE THE X & Y COORDINATES OF THE LATTICE.
      XPOS(1)=0.
      YPOS(JMAX)=0.
      DO 180 I=2, IMAX
  180 XPOS(I)=XPOS(I-1)+XDLT(I)
      DO 190 J=2, JMAX
      JJ=JMAX+1-J
  190 YPOS(JJ)=YPOS(JJ+1)+YDLT(JJ+1)
      GO TO 270
C
C
      INSTRUCTIONS 200 THROUGH 220 ARE A SUBPROGRAM FOR CALCULATING
CC
      THE WIDEST HORMALIZED INCREMENT DLT.
  200 EPSLON=1.-X
      IF(EPSLON.LT.1.E-3) GO TO 210
      DLT=(1.-X)/(1.-X**IMX)
      GQ TO 220
  210 DLT=1.-(IMX-1)*EPSLON/2.
      DLT=1.2(IMX*DLT)
  220 GO TO(100,120,250),KEY
C
      INSTRUCTIONS 230 THROUGH 260 ARE A SUBPROGRAM FOR FINDING DLT
cccc
      USING THE METHOD OF SECANTS.
      FIRST INCREMENT X1 & X2 UNTIL Y1 & Y2 HAVE OPPOSITE SIGNS.
  230 X2=X1-0.02
      Y2=(1.-X2)/(1.-X2**IMX)
      Y2=Y2*X2**(IMX-1)
      Y2=(Y2-CC)/CC
      IF(Y1*Y2.LE.0.) GO TO 240
```

```
X1=X2
Y1=Y2
       GO TO 230
000
       METHOD OF SECANTS
  248 DEN=Y2-Y1
      X=(X1*Y2-X2*Y1)/DEN
       GO TO 200
  250 Y=DLT*X**(IMX-1)
       Y=(Y-CC)/CC
       IF(ABS(Y).LT.0.01) GO TO 260
      X1=X2
       Y1=Y2
      X2=X
      Y2=Y
      GO TO 240
  260 GO TO(140,160),KED
270 RETURN
      END
CC
```

```
SUBROUTINE BORDER
C
00000
      ASSIGNS BOUNDARY CONDITIONS BY MODIFYING THE FINITE-
      DIFFERENCE COEFFICIENTS
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      CONMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XNIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      CONMON/INTGR/IMAX, JMAX, IXNOTH, JYDFTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      CONMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      CIRCLE(X,Y,R)=X*X+Y*Y-R*R
      POINT(Z,R)=SQRT(R*R-Z*Z)
C
      DO 90 I=1, IMAX
      DO 90 J=1, JNAX
      PSI(I,J)=0.
      HDENS(I.J)=0.
      ESUBX(I,J)=0.
      ESUBY(I,J)=0.
   90 IDENT(I, J)=0
      THE LOWER BORDER, WHERE PSI=0
      DO 180 I=1. IMAX
      HSTH( I, 1 )=0.
      HWEST(I,1)=0.
      HCHTR(I,1)=1.E0
      HEAST(I:1)=0.
      HNRTH(I,1)=0.
  100 Q(I,1)=0.
CC
      THE RIGHT BORDER, WHERE PSI=0.
      DO 110 J=1, JMAX
      HSTH(IMAX, J)=0.
      HWEST(IMAX,J)=0.
      HCNTR(IMAX, J)=1.E0
      HEAST(IMAX, J)=0.
      HHRTH(IMAX, J)=0.
  110 Q(IMAX, J)=0.
CCC
      THE UPPER BORDER, WHERE OPSI/DY=0.
      DO 120 I=IXNDTH, IMAX
      HARTH( I . JMAX )=0.
  120 HSTH(I,JMAX)=2.E0*HSTH(I,JMAX)
CC
      THE LEFT BURDER, WHERE DPSI/DX=0.
```

```
DO 130 J=1.JYDPTH
      HWEST(1,J)=0.
  130 HEAST(1,J)=2.E0*HEAST(1,J)
CCC
      THE CORNER REGION
      X0=XPOS(IXWDTH)-RAD
      Y0=YPOS(JYDPTH)-RAD
      I=1
  140 J=JMAX+1
150 J=J-1
      IF (J.LT.JYDPTH)GO TO 180
      IF (XPOS(I).GT.X0)GO TO 170
  160 HSTH(I,J)=0.
      HWEST(I,J)=0.
      HCNTR(I,J)=1.E0
      HEAST(I, J)=0.
      HNRTH(I,J)=0.
      Q(I,J)=1.0
      IDENT(I,J)=-1
      GO TO 150
  170 IF(YPOS(J).LE.Y0)GO TO 160
C
C
      TEST TO DETERMINE IF THE POINT IS EXTERNAL TO THE CIRCLE.
C
      XP=XPOS(I)-X0
      YP=YPOS(J)-Y0
      TSTP=CIRCLE(XP, YP, RAD)
      IF(TSTP.LE.0.)GO TO 160
C
CC
      FIND THE WEST & NORTH DISTANCES TO THE BOUNDARY.
                                                           FIRST
      DETERMINE WHICH POINTS ARE ALSO EXTERNAL, IF ANY.
      XW=XPOS(I-1)-X0
      YN=YPOS(J+1)-Y0
      TSTN=CIRCLE(XW, YP, RAD)
      TSTN=CIRCLE(XP,YN,RAD)
      XW=XPOS(I-1)
      IF(TSTW.LT.0.)XW=X0+POINT(YP,RAD)
      IF(TSTW.LT.0.) IDENT(I,J)=1
      XW=XPOS(I)-XW
      YN=YPOS(J+1)
      IF(TSTN.LT.0.)YN=Y0+P0INT(XP,RAD)
      IF(TSTN.LT.0.) IDENT(I,J)=1
      YN=YPOS(J)-YN
      XWW=XDLT(I)/100.
      YNN=YOLT(J)/100.
      IF(XW.LT.XWW.OR.YN.LT.YNN) GO TO 160
c
      MODIFY HWEST & HNRTH, TO ACCOUNT FOR THE CIRCULAR BOUNDARY.
      XAU=(XDLT(I+1)+XW)/2.E0
      YAU=(YN+YDLT(J))/2.E0
      HWEST(I,J)=YAU/XW
      HNRTH(I,J)=XAUZYN
      HCNTR(I, J)=-(HSTH(I, J)+HWEST(I, J)+HEAST(I, J)+HNRTH(I, J))
```

```
CCCC
      MODIFY GAREA TO ACCOUNT FOR THE PORTION (ASSUMED A
      TRIANGLE) ECLIPSED BY THE CIRCLE.
      X1=XPOS(I)-XDLT(I)/2.E0
      Y1=YPOS(J)-YDLT(J+1)/2.E0
      XP=X1-X0
      YP=Y1-Y0
      TSTP=CIRCLE(XP, YP, RAD)
CCC
      IF (TSTP.GE.0.) NO AREA IS ECLIPSED.
      IF(TSTP.GE.0.)GO TO 150
      Y2=POINT(XP,RAD)+Y0
      X3=POINT(YP,RAD)+X0
      QAREA(I, J)=QAREA(I, J)-(Y2-Y1)*(X3-X1)/2.E0
      GO TO 150
CCC
      INDEX I & CONTINUE UNTIL I.GT. IXWDTH.
  180 I=I+1
      IF(I.LE.IXNDTH) GO TO 140
      IMAXX=IMAX-1
      DO 190 I=1, IMAXX
      00 190 J=2, JMAX
  190 IF(IDENT(I, J).LT.0) PSI(I, J)=1.0
      RETURN
      END
C
C
```

```
SUBROUTINE NITIAL
      PROVIDES INITIAL ESTIMATE FOR PSI(I,J) USING CYLINDRICAL
      COORDINATE DEPLETION THEORY
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONVRG, SIDLT
      COMMON/HRMLZE/DHSHRM, PSINRM, DSTHRM, BLTZMH
CCC
      TRAD=RAD
      TX8=X8
      TY0=Y0
      IF(RAD.GT.0.) GO TO 90
      TRAD=0.05
      TX8=XWIDTH-TRAD
       TY0=YDEPTH-TRAD
   90 IF(RAD.EQ.XWIDTH.AND.RAD.EQ.YDEPTH) GO TO 190
CCCC
      THE HORIZONTAL SHEATH (TAPERED TO MATCH THE RADIAL SOLUTION AT
      THE CIRCULAR CORNER).
  100 RAD1=TRAD+(10.-TRAD)*(TX0-XP0S(I))/TX0
      Y00=YDEPTH-RAD1
      J=JYDPTH
      CALL DEPLTE(X, RAD1)
  110 RD=X*RAD1
  120 J=J-1
      RR=YPOS(J)-Y00
      IF(RR.GE.RD) GO TO 130
      PSI(I,J)=(RR-RD)*(RR+RD)/2.-RD*RD*ALOG(RR/RD)
      GO TO 120
  130 I=I+1
      IF(XPOS(I).GT.TX0) GO TO 140
      GO TO 100
      THE VERTICAL SHEATH (TAPERED IN THE SAME MANNER).
C
  140 IM=I-1
      J=JNAX
  150 RAD1=TRAD+(10.-TRAD)*(TY0-YPOS(J))/TY0
      X00=XWIDTH-RAD1
      I = I \times WDTH
      CALL DEPLTE(X, RAD1)
  160 RD=X*RAD1
  170 I=I+1
      RR=XPOS(I)-X00
```

```
IF(RR.GE.RD) GO TO 180
      PSI(I,J)=(RR-RD)*(RR+RD)/2.-RD*RD*ALOG(RR/RD)
      GO TO 170
  180 J=J-1
      IF(YPOS(J).GT.TY0) GO TO 200
      GO TO 150
  190 I=0
      J=JMAX
      GO TO 210
  200 I=IM
  210 RAD1=TRAD
C
CC
      THE CIRCULAR CORNER SHEATH
      CALL DEPLTE(X, RAD1)
  220 RD=X*RAD1
  230 I=I+1
      XP=XPOS(I)-TX0
      YP=YPOS(J)-TY0
      RR=SQRT(XP*XP+YP*YP)
      IF(RR.LE.RAD1) GO TO 230
      IF(RR.GE.RD) GO TO 240
      PSI(I,J)=(RR-RD)*(RR+RD)/2.-RD*RD*ALOG(RR/RD)
      GO TO 230
  240 J=J-1
      YP=YPOS(J)-TY0
      IF(YP.GE.RD) RETURN
      IF(RAD.EQ.XWIDTH.AND.RAD.EQ.YDEPTH) GO TO 250
      I = IM
      GO TO 230
  250 I=0
      GO TO 230
      END
```

```
SUBROUTINE DEPLTE(X, RAD1)
C
CCC
      FINDS THE DEPLETION RADIUS FROM A 1-D SOLUTION OF POISSON'S
      EQUATION IN CYLINDRICAL COORDINATES. RETURNS X=RD/RAD1
      RHS(X)=1.-RAD1*RAD1*((1.-X*X)/2.+X*X*AL0G(X))
ccccc
      FOR RADI .GT. 0.3. THE METHOD OF SECANTS IS USED TO FIND X.
      FOR RADI .LT. 0.3. A METHOD OF SUCCESSIVE APPROXIMATIONS WHICH
      IS VERY FAST IS USED. (THE LATTER FAILS TO CONVERGE WHEN RAD)
      EXCEEDS 0.5.)
       IF(RAD1.GT.0.3) GO TO 110
      X1=(3.+4. *RAD1)/(4. *RAD1)
  100 X=SQRT((2./(RAD1*RAD1)-1.)/(2.*ALOG(X1)-1.))
      Y=RHS(X)
      IF(ABS(Y).LT.1.E-3) RETURN
      11=1
      GO TO 100
C
      METHOD OF SECANTS. FIRST FIND X1 & X2 CAUSING Y1 & Y2 TO HAVE OPPOSITE SIGNS. THE STARTING POINT FOR X1 DIFFERS WHEN RAD1 .GT.
C
C
C
      0.9. BASED ON EMPIRICAL KNOWLEDGE OF THE APPROXIMATE VALUE OF
C
      THE ROOT TO SPEED UP THE SEARCH.
  110 IF(RAD1.GT.0.9) GO TO 120
      X1=4
      Y1=RHS(X1)
      GO TO 130
  120 X1=2
      Y1=RHS(X1)
  130 N2=N1-0.1
      Y2=RHS(X2)
      YY=Y1*Y2
      IF(YY.LT.0) GO TO 140
      X1=X2
      Y1=Y2
      GO TO 130
  140 X=(X1*Y2-X2*Y1)/(Y2-Y1)
      Y=RHS(X)
      IF(ABS(Y).LT.1.E-3) RETURN
      X1=X2
      Y1=Y2
      X5=X
      1.5=1.
      GO TO 140
```

END

```
SUBROUTINE GRELAX
CCCC
      IMPLEMENTS GUMMEL'S RELAXATION ALGORITHM FOR PSI
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      CONMON/CDEFF/HSTH(31.31).HWEST(31.31).HCNTR(31.31).HEAST(31.31).
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH. YDEPTH. BRRIER. EGAP, TMPTR. ACCPTR. UBLTIN, UOLT,
     &TRHSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, INNOTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      OMEGA=1.6
      IT=1
      IMAXX=IMAX-1
  100 DL TMX=0
      CALL DNSITY
      CALL POISSN
      00 110 I=1. IMAXX
      00 110 J=2 JMAX
      DLTMX=AMAX1(ABS(DELTA(I,J)),DLTMX)
      PSI(I,J)=PSI(I,J)+OMEGA*DELTA(I,J)
      IF(PSI(I,J),LT,\theta,) PSI(I,J)=\theta.
  110 CONTINUE
      DMX=0
      00 500 I=1 IMANN
      DO 500 J=2. JMAX
      IF(ABS(DELTA(I,J)).LE.DMX) GO TO 500
      DNX=ABS(DELTA(I,J))
      II=I
      JJ=J
  500 CONTINUE
      WRITE(6,5000) DELTA(II,JJ),II,JJ
 5000 FORMAT(1H0,5%, 'MAX DELTA IN GRELAX IS', 1PE11.3,1%,
     &'AT COORDINATE (', 12, ', ', 12, ')')
      IF(DLTMX.LE.CONURG) GO TO 120
      IT=IT+1
      IF(IT.GT.ITMAX) GO TO 130
      GO TO 100
  120 WRITE(6, 1000) IT
                            ITERATIONS WERE REQUIRED IN GRELAX'. ///
 1000 FORMAT(1H0,5%, I5, '
      RETURN
  130 WRITE(6,1010) DLTMX, CONURG
 1010 FORMAT(1H0,5%, 'MAXIMUM ITERATIONS WERE EXCEEDED IN &GRELAX. DLTMX=',1PE10.2,' CONURG=',1PE10.2,'/)
      STOP
      END
```

CC

```
SUBROUTINE POISSN
0000
      SOLVES POISSONS EQUATION USING STONES METHOD.
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEFTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC.QSS.X0.Y0.RAD.XDELTA.YDELTA
      COMMON/INTGR/INAX, JMAX, IXNOTH, JYDFTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONVRG, SIDLT
      COMMON/HRMLZE/DHSHRM, PSIHRM, DSTHRM, BLTZMH
C
      DIMENZR: TZRGEW(31,31)
      DO 100 I=1 IMAX
      00 100 J=1. JMAX
      PSINEW(I,J)=PSI(I,J)
      B(I,J)=HSTH(I,J)
      D(I,J)=HWEST(I,J)
      E(I,J)=HCNTR(I,J)
      F(I,J)=HEAST(I,J)
  100 H(I,J)=HNRTH(I,J)
      CALL CHARGE
      ITERATIVE STONE'S METHOD
      ISTONE=0
      ITR=1
  110 ISTONE=ISTONE+1
      CALL STONE(ISTONE, IMAX, JMAX, RESID, PSINEW)
      IF(RESID.LE.SIDLT) GO TO 120
      ITR=ITR+1
      IF(ITR.LE.ITRMAX) GO TO 110
      WRITE(6, 1000)
 1000 FORMAT(1H0.1X, 'MAXIMUM ITERATIONS EXCEEDED IN POISSN'./)
      STOP
  120 00 130 I=1, IMAX
      DO 130 J=1, JMAX
  130 DELTA(I,J)=PSINEW(I,J)-PSI(I,J)
      WRITE(6,5000) ITR
 5000 FORMAT(2X,//,2X,I5,1X,'ITERATIONS WERE REQUIRED WITH STONES METHOD
     &IN POISSN')
      RETURN
      END
```

END

```
SUBROUTINE CHARGE
00000
      CALCULATES THE CHARGE TERMS IN GUMNELS ALGORITHM
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      CONMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMON/INTGR/INAX, JNAX, IXWDTH, JYDPTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      ALPHA=PSINRM/BLTZMN
      IMAXX=IMAX-1
      00 100 I=1. IMAXX
      DO 100 J=2, JMAX
      IF(IDENT(I,J).LT.0) GO TO 100
      Q(I,J)=1.+EDENS(I,J)-HDENS(I,J)-ALPHA*(EDENS(I,J)+HDENS(I,J))*
     \&PSI(I,J)
      Q(I,J)=2.*Q(I,J)*QAREA(I,J)
      E(I,J)=E(I,J)-2.*(EDENS(I,J)+HDENS(I,J))*ALPHA*QAREA(I,J)
  100 CONTINUE
C
      MODIFY Q AT THE UPPER BORDER TO INCLUDE SURFACE CHARGE QSS.
      II=IXWDTH+1
      00 110 I=II. IMAX
  110 Q(I,JMAX)=Q(I,JMAX)-QSS*(XDLT(I)+XDLT(I+1))
      RETURN
      END
CC
```

U(1,1)=R/DD

```
IF(ABS(U(1,1)).LT.1.E-7) U(1,1)=0.
CCC
      THE ROW K=1. EXCLUDING THE RIGHT CORNER POINT.
      DO 100 J=2, JMAXX
      JP=J+1
      JN=J-1
      CC=CN(D(J,1),FF(JN,1))
      DD=E(J,1)+DN2(FF(JN,1),EE(JN,1))
      EE(J,1)=F(J,1)/DD
      FF(J,1)=FN(H(J,1),FF(JN,1))
      R=Q(J,1)+(D(J,1)*T(JN,1)+E(J,1)*T(J,1)+F(J,1)*T(JP,1)+H(J,1)*
     &T(J,2))
      RR=ABS(R)
      IF (RR.GT.RESID) RESID=RR
      U(J,1)=(R-CC*U(JN,1))/DD
  100 IF(ABS(V(J,1)).LT.1.E-7) V(J,1)=0.
CCC
      THE CORNER POINT (JMAX,1)
      J=JMAX
      XXAML=HL
      CC=CN(D(J,1),FF(JN,1))
      DD=E(J,1)+DN2(FF(JN,1),EE(JN,1))
      EE(J. 1)=0.
      FF(J,1)=FN(H(J,1),FF(JN,1))
      R=Q(J,1)-(D(J,1)*T(JN,1)+E(J,1)*T(J,1)+H(J,1)*T(J,2))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      V(J,1)=(R-CC*V(JN,1))/DD
      IF(ABS(U(J,1)).LT.1.E-7) U(J,1)=0.
C
C
      ALL ROWS EXCEPT ROW KMAX
      DO 120 K=2,KMAXX
      KP = K + 1
      KH=K-1
C.
C
      THE LEFT BURDER POINT
      BB=BH(B(1,K),EE(1,KH))
      DO=E(1,K)+DN1(EE(1,KN),FF(1,KN))
      EE(1,K)=EN(F(1,K),EE(1,KN))
      FF(1,K)=H(1,K)/DD
      R=Q(1,K)-(B(1,K)*T(1,KN)+E(1,K)*T(1,K)+F(1,K)*T(2,K)+H(1,K)*
     &T(1,KP>)
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(1,K)=(R-BB*U(1,KN))/DD
      IF(ABS(U(1,K)).LT.1.E-7) U(1,K)=0.
      THE ROW K EXCLUDING THE RIGHT BORDER POINT.
      DO 110 J=2, JMAXX
      JP = J + 1
      JH=J-1
```

```
BB=BN(B(J,K),EE(J,KN))
      CC=CN(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J,K)=EN(F(J,K),EE(J,KN))
      FF(J,K)=FN(H(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)+
     &F(J,K)*T(JP,K)+H(J,K)*T(J,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
  110 IF(ABS(V(J,K)).LT.1.E-7) U(J,K)=0.
CC
      THE RIGHT BURDER FOINT
      J=JMAX
      XXANL=NL
      BB=BN(B(J,K),EE(J,KN))
      CC=CH(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J,K)=0
      FF(J,K)=FN(H(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)+H(J,K)*
     &T(J,KP))
      RR=ABS(R)
      IF (RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
  120 IF(ABS(V(J,K)).LT.1.E-7) V(J,K)=0.
CCC
      THE CORNER POINT (1,KMAX)
      K=KMAX
      KH=KMAXX
      BB=BN(B(1,K),EE(1,KN))
      DD=E(1,K)+DN1(EE(1,KN),FF(1,KN))
      EE(1,K)=EN(F(1,K),EE(1,KN))
      FF(1,K)=0
      R=Q(1,K)-(B(1,K)*T(1,KN)+E(1,K)*T(1,K)+F(1,K)*T(2,K))
      RR = ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(1,K)=(R-BB*U(1,KN))/DD
      IF(ABS(U(1,K)).LT.1.E-7) U(1,K)=0.
CC
      THE ROW KMAX, EXCLUDING THE CORNER POINT (JMAX,KMAX)
      DO 130 J=2, JMAXX
      JP = J + 1
      JN = J - 1
      BB=BN(B(J,K),EE(J,KN))
      CC=CH(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J,K)=EN(F(J,K),EE(J,KN))
      FF(J,K)=\emptyset
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)*T(J,K)+F(J,K)*
     &T(JP,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
```

```
U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
  130 IF(ABS(U(J,K)).LT.1.E-7) U(J,K)=0.
C
CC
      THE CORNER POINT (JMAX, KMAX)
      J=JMAX
      XXANL=NL
      BB=BN(B(J,K),EE(J,KN))
      CC=CN(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J,K)=0
      FF(J,K)=0
      R=R(J_1K)+(B(J_1K)*T(J_1KN)+B(J_1K)*T(JN_1K)+E(J_1K)*T(J_1K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      V(J,K)=(R-BB*V(J,KN)-CC*V(JN,K))/DD
      IF(ABS(U(J_iK)),LT,1,E-7),U(J_iK)=0.
00000
      INDEX K AND J IN REVERSE TO FIND DELTA
      THE CORNER POINT (JNAX, KNAX)
C
      K=KMAX
      DELTA( JMAX, K )=U( JMAX, K )
CC
      THE ROW KMAX
      DO 148 JJ=1, JNAXX
      J=JMAXX+1-JJ
      JP=J+1
      DELTA(J,K)=U(J,K)-EE(J,K)*DELTA(JP,K)
  140 IF(ABS(DELTA(J,K)).LT.1.E-10) DELTA(J,K)=0.
CCC
      THE ROW K. TREATING THE RIGHT BORDER FIRST.
      00 150 KK=1 KMAXX
      K=KMAXX+1-KK
      KP = K + 1
      DELTA(JMAX,K)=U(JMAX,K)-FF(JMAX,K)*DELTA(JMAX,KF)
      IF(ABS(DELTA(JMAX,K)).LT.1.E-10) DELTA(JMAX,K)=0.
      DO 150 JJ=1, JMAXX
      J=JMAXX+1-JJ
      JP=J+1
      DELTA(J,K)=U(J,K)-EE(J,K)*DELTA(JP,K)-FF(J,K)*DELTA(J,KP)
  150 IF(ABS(DELTA(J,K)).LT.1.E-10) DELTA(J,K)=0.
      GO TO 240
00000
      ISTONE IS EVEN.
                        INDEX K IN REVERSE ORDER.
      THE CORNER POINT (1,KMAX)
  170 K=KMAK
      KH=KMAXX
      DD=E(1,K)
      EE(1,K)=F(1,K)/00
      FF(1,K)=B(1,K)/DD
```

```
R=Q(1,K)-(B(1,K)*T(1,K))+E(1,K)*T(1,K)+F(1,K)*T(2,K))
      RR=ABS(R)
      RESID=RR
      U(1,K)=R/DD
      IF(ABS(U(1,K)),LT,1,E-7) U(1,K)=0.
      THE RON KMAX
      DO 180 J=2, JMAXX
      JP=J+1
      JN=J-1
      CC=CR(D(J,K),FF(JN,K))
      DD=E(J,K)+DR2(FF(JN,K),EE(JN,K))
      EE(J,K)=F(J,K)/DD
      FF(J_{\lambda}K)=FR(B(J_{\lambda}K)_{\lambda}FF(JN_{\lambda}K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)+F(J,K)*
     &T(JP,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-CC*U(JN,K))/DD
  180 IF(ABS(U(J,K)).LT.1.E-7) U(J,K)=0.
      THE CORNER POINT (JMAX, KMAX)
      J=JMAK
      JN=JMAXX
      CC=CR(D(J,K),FF(JH,K))
      DD=E(J,K)+DR2(FF(JN,K),EE(JN,K))
      EE(J,K)=0
      FF(J,K)=FR(B(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-CC*U(JN,K))/DD
      IF(ABS(U(J,K)).LT.1.E-7) U(J,K)=0.
      ALL RONS EXCEPT THE ROW K=1
      00 208 KK=2 KMAXX
      K=KMAXX+2-KK
      KP=K+1
      KN=K-1
CC
      THE LEFT BORDER POINT (1.K)
      BB=BR(H(1,K),EE(1,KP))
      DD=E(1,K)+DR1(EE(1,KP),FF(1,KP))
      EE(1,K)=ER(F(1,K),EE(1,KF))
      FF(1,K)=B(1,K)/DD
      R=Q(1,K)-(B(1,K)*T(1,KN)+E(1,K)*T(1,K)+F(1,K)*T(2,K)+H(1,K)*
     &T(1,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(1,K)=(R-BB*U(1,KP))/DD
      IF(ABS(U(1,K)).LT.1.E-7) U(1,K)=0.
C
```

```
CC
       THE ROW K EXCLUDING THE RIGHT BORDER POINT
      00 190 J=2, JMAXX
       JP=J+1
       JH=J-1
      B8=BR(H(J,K),EE(J,KP))
      CC=CR(D(J,K),FF(JN,K))
      DD=E(J,K)+DR1(EE(J,KP),FF(J,KP))+DR2(FF(JN,K),EE(JN,K))
      EE(J,K)=ER(F(J,K),EE(J,KP))
      FF(J,K)=FR(B(J,K),FF(JN,K))
      R=Q(J_*K)+(B(J_*K)*T(J_*KN)+D(J_*K)*T(JN_*K)+E(J_*K)*T(J_*K)+F(J_*K)*
     &T(JP,K)+H(J,K)*T(J,KP))
      RR=ABS(R)
       IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KP)-CC*U(JN,K))/DD
  190 IF(ABS(V(J,K)),LT.1.E-7) V(J,K)=0.
C
C
      THE RIGHT BORDER POINT
0
      J=JMAX
      JN=JMAXX
      BB=BR(H(J,K),EE(J,KP))
      CC=CR(D(J,K),FF(JN,K))
      DD=E(J,K)+DR1(EE(J,KP),FF(J,KP))+BR2(FF(JN,K),EE(JN,K))
      EE(J,K)=0
      FF(J,K)=FR(B(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)+H(J,K)*
     &T(J,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-88*U(J,KP)-CC*U(JN,K))/DD
  200 IF(ABS(V(J,K)).LT.1.E-7) V(J,K)=0.
C
C
      THE CORNER POINT (1,1)
C
      BB=BR(H(1,1),EE(1,2))
      DD=E(1,1)+DR1(EE(1,2),FF(1,2))
      EE(1,1)=ER(F(1,1),EE(1,2))
      FF(1,1)=0.
      R=R(1,1)-(E(1,1)*T(1,1)+F(1,1)*T(2,1)+H(1,1)*T(1,2))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      V(1,1)=(R-BB*V(1,2))/DD
      IF(ABS(U(1,1)).LT.1.E-7) U(1,1)=0.
CC
      THE ROW K=1, EXCLUDING THE RIGHT CORNER POINT.
      DO 210 J=2, JMAXX
      JP=J+1
      JN=J-1
      BB=BR(H(J,1),EE(J,2))
      CC=CR(O(J,1),FF(JN,1))
      DD=E(J,1)+DR1(EE(J,2),FF(J,2))+DR2(FF(JN,1),EE(JN,1))
      EE(J,1)=ER(F(J,1),EE(J,2))
      FF(J,1)=0
      R=R(J,1)-(D(J,1)*T(JN,1)+E(J,1)*T(J,1)+F(J,1)*T(JP,1)+H(J,1)*
     &T(J,2))
```

```
RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,1)=(R-BB\U(J,2)-CC\U(JN,1))/DD
  210 IF(ABS(V(J,1)).LT.1.E-7) V(J,1)=0.
0000
      THE CORNER POINT (JNAX,1)
      XAML=L
      XXAML=NL
      BB=BR(H(J,1),EE(J,2))
      CC=CR(D(J,1),FF(JN,1))
      DD=E(J,1)+DR1(EE(J,2),FF(J,2))+DR2(FF(JN,1),EE(JN,1))
      EE(J,1)=8.
      FF(J.1)=0.
      R=R(J,1)-(D(J,1)*T(JN,1)+E(J,1)*T(J,1)+H(J,1)*T(J,2))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,1)=(R-BB*U(J,2)-CC*U(JN,1))/DD
      IF(ABS(U(J,1)).LT.1.E-7) U(J,1)=0.
CCCC
      INDEX K FORWARD & J REVERSE TO FIND DELTA
      THE POINT (JMAX, 1)
C
      DELTACINAX, 1 >=UCJNAX, 1 >
C
C
      THE ROW K=1
      DO 220 JJ=1,JMAXX
      UL-I+XXANL=L
      JF = J+1
      DELTA(J,1)=U(J,1)-EE(J,1)*DELTA(JP,1)
  220 IF(ABS(DELTA(J,1)).LT.1.E-10) DELTA(J,1)=0.
CC
      ALL REMAINING ROWS
C
      DO 230 K=2,KMAX
      KH = K - 1
CCC
      THE RIGHT BORDER POINT
      DELTA(JMAX,K)=U(JMAX,K)-FF(JMAX,K)*DELTA(JMAX,KN)
      IF(ABS(DELTA(JMAX,K)).LT.1.E-10) DELTA(JMAX,K)=0.
C
C
      ALL REMAINING POINTS OF THE ROW
      DO 238 JJ=1,JMAXX
      J=JMAXX+1-JJ
      JP=J+1
      DELTA(J,K)=U(J,K)-EE(J,K)*DELTA(JP,K)-FF(J,K)*DELTA(J,KN)
  230 IF(ABS(DELTA(J,K)).LT.1.E-10) DELTA(J,K)=0.
C
      CALCULATE NEW T(J,K)
  240 DO 250 J=1, JMAX
      DO 250 K=1.KMAX
```

```
250 T(J,K)=T(J,K)+DELTA(J,K)
      RETURN
C
CC
      ENTRY STONE1 SETS UP ALPHA VALUES & INITIALIZES ALL ARRAYS
      ENTRY STONE 1 (JMAX, KMAX)
C
      00 320 J=2, JMAX
      DO 320 K=2,KMAX
      DX=XDLT(J)/XPOS(JMAX)
      DY=YDLT(K)/YPOS(1)
  320 EE(J,K)=2.E0/(1.E0/(DX*DX)+1 E0/(DY*DY))
CCC
      FIND AVERAGE
      ALPHX=0
      DO 330 J=2, JMAX
      DO 330 K=2,KMAX
  330 ALPHX=ALPHX+EE(J,K)
      ALPHX=ALPHX/(JMAX*KMAX)
000
      IMPLEMENT STONE'S EQ(27)
      DO 340 J=1,9
      ALPHY=J-1
      ALPHY=ALPHY/8.E0
  340 EE(J,1)=ALPHX**ALPHY
CCC
      IMPLEMENT THE SEQUENCE OF 18 ALPHAS SUGGESTED BY STONE
      ALPHA(1)=EE(9,1)
      ALPHA(3)=EE(6,1)
      ALPHA(5)=EE(3,1)
      ALPHA(7)=EE(8,1)
      ALPHA(9)=EE(5,1)
      ALPHA(11)=EE(2,1)
      ALPHA(13)=EE(7,1)
      ALPHA(15)=EE(4,1)
      ALPHA(17)=EE(1,1)
      00 350 J=2,18,2
  350 ALPHA(J)=ALPHA(J-1)
      DO 360 J=1,18
  360 ALPHA(J)=1.E0-ALPHA(J)
00000
      INITIALIZE ALL ARRAYS INTERNAL TO STONE TO ZERO.
      00 370 J=1. JMAX
      00 370 K=1 KMAX
      EE(J,K)=0.
      FF(J,K)=0.
      U(J,K)=0
  370 DELTA(J.K)=0.
      RETURN
      END
C
```

```
SUBROUTINE EFIELD
CCCC
      CALCULATES THE ELECTRIC FIELD COMPONENTS ESUBX & ESUBY
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
     COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31), &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX.JMAX.IXWDTH.JYDPTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
CCC
      ESUBX COMPONENT
      IMAXX=IMAX-1
      00 140 I=2, IMAXX
      00 140 J=2, JMAX
      XW=XDLT(I)
      IF(IDENT(I,J).LT.0) GO TO 140
      IF(IDENT(I,J),EQ.0) GO TO 120
      IF(J.EQ.JMAX) GO TO 100
      YAU=(YDLT(J+1)+YDLT(J))/2.E0
      GO TO 110
  100 YAU=YDLT(J)
  110 XW=YAU/HWEST(I,J)
  120 ESUBX([,J)=((PSI([,J)-PSI([+1,J))/XDLT([+1)+(PSI([-1,J)-PSI([,J))
     &/XW)/2.E0
  140 CONTINUE
CC
      ESUBY COMPONENT
       JMAXX=JMAX-1
      DO 190 I=1, IMAXX
DO 190 J=2, JMAXX
      YN=YDLT(J+1)
      IF(IDENT(I,J).LT.0) GO TO 190
      IF(IDENT(I, J).EQ.0) GO TO 170
      IF(I.EQ.1) GO TO 150
      XAU=(XDLT(I)+XDLT(I+1))/2.E0
      GO TO 160
  150 XAU=XDLT(2)
  160 YM=XAU/HNRTH(I,J)
  170 ESUBY([,J)=((PSI([,J+1)-PSI([,J))/YN+(PSI([,J)-PSI([,J-1))/
     &YOLT(J))/2.E0
  190 CONTINUE
      APPLY QUADRATIC EXTRAPOLATION TO FILL IN ESUBX & ESUBY AT THE
000
      EXTERNAL POINTS BORDERING THE INTERFACE.
      DO 200 I=1, IMAX
      DO 200 J=1, JMAX
```

```
IF(IDENT(I,J).GE.0) GO TO 200
    IF(IDENT(I+1, J).LT.0) GO TO 200
    DENOM=XDLT(I+3)*XDLT(I+2)*(XDLT(I+3)+XDLT(I+2))
    XX=XDLT(I+2)+XDLT(I+1)
    DENUM=XDLT(I+2)*ESUBX(I+3,J)+XDLT(I+3)*ESUBX(I+1,J)-
   &(XDLT(I+2)+XDLT(I+3))*ESUBX(I+2,J)
    AA=DENUM/DENOM
    DENUM=XDLT(I+2)*XDLT(I+2)*ESUBX(I+3,J)-XDLT(I+3)*XDLT(I+3)*
   &ESUBX(I+1,J)-(XDLT(I+2)*XDLT(I+2)-XDLT(I+3)*XDLT(I+3))*
   &ESUBX(I+2,J)
    BB=DENUM/DENOM
    ESUBX(I,J)=ESUBX(I+2,J)+AA*XX*XX-BB*XX
    DENOM=YOLT(J-2)*YOLT(J-1)*(YOLT(J-2)+YOLT(J-1))
    XX=YDLT(J-1)+YDLT(J)
    DENUM=YOLT(J-1)*ESUBY(I,J-3)+YOLT(J-2)*ESUBY(I,J-1)-
   &(YDLT(J-1)+YDLT(J-2))*ESUBY(I,J-2)
    AA=DENUM/DENUM
    DEMUM=YDLT(J-1)*YDLT(J-1)*ESUBY(I,J-3)-YDLT(J-2)*YDLT(J-2)*
   &ESUBY(I,J-1)-(YDLT(J-1)*YDLT(J-1)-YDLT(J-2)*YDLT(J-2))*
   &ESUBY(I, J-2)
    BB=DENUM/DENOM
    ESUBY(I,J)=ESUBY(I,J-2)+AA*XX*XX-BB*XX
200 CONTINUE
    RETURN
    END
```

SE

```
CC
      SUBROUTINE AVENCH (VETDET, AVDET, XPATH, YPATH, ET, KNTMAX)
coccocc
      EVALUATES THE BREAKDOWN VOLTAGE AFTER LOCATING THE TRAJECTORY
      ALONG WHICH THE IONIZATION INTEGRAL IS A MAXIMUM.
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XNIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMON/INTGR/IMAX, JMAX, IXNOTH, JYDFTH
      COMMON/COTTRL/ITMAX, ITTMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
      COMMON/SNGLE/VOLTO, DLTVLT, NVOLT, KOUTPT
      COMMON/RSCALE/ RSFCTR
      DIMENSION XSTART(3), YSTART(3), PI(3), KNTMX(3), ISTART(3), JSTART(3)
      DIMENSION XPATH(KNTMAX,3),YPATH(KNTMAX,3),ET(KNTMAX,3)
      DIMENSION RR(3), OMEG(3)
CCCC
      CALCULATE EQUILIBRIUM PARAMETERS. ESTIMATE THE BREAKDOWN VOLTAGE.
      AND CALCULATE INITIAL NORMALIZATIONS.
      CALL EQULIB
      RSFCTR=1.0
      RDSAUE=RAD
      XWSAUE=XWIDTH
      YDSAVE=YDEPTH
      QSSAVE=QSS
      VOLT≈VOLT0-DLTVLT
      N=B
   90 N=N+1
      IF(N.GT.NUOLT) RETURN
      VOLT≈VOLT+DLTVLT
      PSINRM=UBLTIN+UOLT
      DSTHRM=SQRT(2.*11.7*8.854E-14*PSINRM/(1.602E-19*DNSNRM))
IF(RDSAUE.NE.XWSAUE.OR.RDSAUE.NE.YDSAUE) GO TO 95
      RAD1=RDSAUE/(DSTNRM*1.E4)
      CALL DEPLIE(X, RAD1)
      RD=X*RAD1
      RSFCTR=RO-RAD1
   95 KSWCH=0
      K=1
      ISTART(2)=IXWDTH
      JSTART(2)=JYDPTH
CCC
```

85

PROVIDE CURRENT NORMALIZATIONS OF RAD, XNIDTH, YDEPTH, & QSS

100 RAD=RDSAVE/(DSTNRM\*1.E4)

```
XWIDTH=XWSAUE/(DSTNRM*1.E4)
      YDEPTH=YDSAUE+CDSTNRM*1.E4)
      QSS=QSSAUE*DSTNRM/(11.7*8.854E-14*PSINRM)
      SINRM@=PSINRM
0000000
      USING PRESENT NORMALIZATIONS, SOLVE POISSON'S EQ. & OBTAIN THE
      ELECTRIC FIELD LATTICES. IF KSNCH.EQ.O, LOCATE POSITION OF MAX
      E-FIELD AND ESTABLISH THREE STARTING LOCATIONS CENTERED ABOUT THAT
      POSITION. IF KSWCH.GT.0, ESTABLISH ONLY THE CENTRAL STARTING
      LOCATION.
      CALL GRID
      CALL STONE ((IMAX, JMAX)
      CALL BORDER
      CALL NITIAL
      CALL GRELAX
      CALL EFIELD
      I=ISTART(2)-1
      J=JSTART(2)-1
      IF(RAD.NE.XWIDTH.OR.RAD.NE.YDEPTH.OR.QSS.NE.0.) GO TO 105
      K=2
      KSWCH=1
      GO TO 120
  105 IF(KSNCH.GT.0) GO TO 120
      ETST=2.E5*DSTNRM/PSINRM
      EMAX=0.
      00 110 II=1, IMAX
      00 110 JJ=1, JMAX
      ETT=SQRT(ESUBX(II, JJ)*ESUBX(II, JJ)+ESUBY(II, JJ)*ESUBY(II, JJ))
      IF(ETT.LE.EMAX) GO TO 110
      ENAX=ETT
      I = II
      J=JJ
  110 CONTINUE
      IF(EMAX.GE.ETST) GO TO 115
      EMAX=EMAX*PSINRM/DSTNRM
      WRITE(6,1040) UOLT, EMAX
 1040 FORMAT(1H0,5%, 'SKIPPING VOLT=',1PE10.2,' . MAX ELECTRIC FIELD
     &TOO SMALL (ENAX=',1PE10.2,')')
      GO TO 90
  115 I=I-2
      J=J-2
CC
      ESTABLISH STARTING COORDINATES FOR TRAJECTORY K.
C
  120 I=I+1
      J=J+1
      X=XPOS(I)
      Y=YPOS(J)
      IF(X.GT.X0) GO TO 125
      XSTART(K)=X
      YSTART(K)=YPOS(JYDPTH)
      GO TO 150
  125 IF(Y.GT.Y0) GO TO 130
      XSTART(K)=XPOS(IXWDTH)
      YSTART(K)=Y
```

```
GO TO 150
  130 X=X-X0
       Y=Y-Y0
       IF(X.LT.Y) GO TO 140
       Y=Y/X
      XSTART(K)=X0+RAD/SQRT(1.E0+Y*Y)
       YSTART(K)=Y0+(XSTART(K)-X0)*Y
      GO TO 150
  148 X=X/Y
       YSTART(K)=Y0+RAD/SQRT(1.E0+X*X)
      XSTARI(K)=X0+(YSTARI(K)-Y0)*X
  150 IF(KSNCH.GT.0) GO TO 180
      K=K+1
       IF(K.GT.3) GO TO 170
      GO TO 120
C
       TRACE OUT THE TRAJECTORY FOR STARTING POSITION K.
  170 K=1
  180 KNT=1
      KEXIT=0
      X=XSTART(K)
      Y=YSTART(K)
      I = IXWOTH
      J=JYDPTH
      DLTX=X-XPOS(IXWDTH)
      DLTY=Y-YPOS(JYDPTH)
      CALL INDEX(I) J. DLTX, DLTY, KEXIT)
      ISTART(K)=I
      JSTART(K)=J
      IF(DLTX.LT.XDLT(I+1)/1.E3) DLTX=XDLT(I+1)/1.E3
      IF(DLTY.LT.YDLT(J)/1.E3) DLTY=YDLT(J)/1.E3
      X=XPOS(I)+DLIX
      Y=YPOS(J)+DLTY
      CALL EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET(1, K))
      XPATH(1,K)=X
      YPATH(1,K)=Y
      ETT=ET(1,K)
  190 CALL TRAJEC(KNT, I, J, X, Y, DLTX, DLTY, ETT, KEXIT)
      IF(KEXIT.GT.0) GO TO 200
      KNT=KNT+1
      IF(KNT.GT.KNTMAX) GO TO 195
      XPATH(KNT,K)=X
      YPATH(KNT,K)=Y
      ET(KNT,K)=ETT
      GO TO 190
  195 WRITE(6,1000) KNTMAX
 1000 FORMAT(1H1,30X,/,5X,'EXCEEDED STORAGE ALLOTTED FOR TRAJECTORIES '
     &'(KNTMAX=',13,').',/,5X,'INCREASE THE VALUE OF THAT PARAMETER ',
&'IN HAMELIST CONTRL.',/,5X,'INCREASE DIMENSIONS ',
     &'ALLOTED TO XPATH, YPATH, & ET IN MAIN, IF NECESSARY.')
      STOP
  200 KHTMX(K)=KHT
C
      APPLY PARABOLIC EXTRAPOLATION TO OBTAIN A BETTER ESTIMATE OF
      ET(1,K) AT THE INTERFACE.
```

```
C
      DX=XPATH(4,K)-XPATH(3,K)
      DY=YPATH(4,K)-YPATH(3,K)
      DSP=SQRT(DX*DX+DY*DY)
      DX=XPATH(3,K)-XPATH(2,K)
      DY=YPATH(3,K)-YPATH(2,K)
      DSN=SQRT(DX*DX+DY*DY)
      DX=XPATH(3,K)-XPATH(1,K)
      DY=YPATH(3,K)-YPATH(1,K)
      DS=SQRT(DX*DX+DY*DY)
      DENOM=DSP*DSN*(DSP+DSN)
      DENUM=DSN*ET(4,K)+DSP*ET(2,K)-(DSP+DSN)*ET(3,K)
      AA=DENUM/DENOM
      DENUM=DSN*DSN*ET(4,K)-DSP*DSP*ET(2,K)-(DSN*DSN-DSP*DSP)*ET(3,K)
      BB=DENUM/DENOM
      ET(1,K)=ET(3,K)+AA*DS*DS-BB*DS
      KNT=1
      PI(K)=0.
      RR(K)=0.
      OMEG(K)=0
      XPT=XPATH(1,K)*DSTNRM*1.E4
      YPT=YPATH(1,K)*DSTNRN*1.E4
      EPT=ET(1,K)*PSINRM/DSTNRM
      WRITE(6,1010) K, ISTART(K), JSTART(K), XPT, YPT, EPT, PI(K), OMEG(K)
 1010 FORMAT(2X,//,2X,'K',3X,'ISTART',1X,'JSTART',3X,'XPATH',5X,
&'YPATH',7X,'ET',6X,'ALPHN',5X,'ALPHP',6X,'PI',7X,'OMEGA',
     &//, 1X, I2, 5X, I2, 5X, I2, 3X, 1P3E10.2, 20X, 1P2E10.2)
CC
      EVALUATE THE IONIZATION INTEGRAL ALONG TRAJECTORY K.
  210 KNT=KNT+1
      IF(KNT.GT.KNTMX(K)) GO TO 220
      DX=XFATH(KNT,K)-XPATH(KNT-1,K)
      DY=YPATH(KNT,K)-YPATH(KNT-1,K)
      ET2=ET(KNT,K)
      ET1=ET(KNT-1,K)
      ONEGO=ONEG(K)
      CALL JNTGRL(DX,DY,ET1,ET2,PI(K),RR(K),OMEG(K),ALPHN,ALPHP)
      XPT=XPATH(KNT,K)*DSTNRM*1.E4
      YPT=YPATH(KNT,K)*DSTNRM*1.E4
      EPT=ET(KNT,K)*PSINRM/DSTNRM
      WRITE(6,1020) XPT, YPT, EPT, ALPHN, ALPHP, PI(K), OMEG(K)
 1020 FORMAT(20X, 1P7E10.2)
      TST≈(OMEG(K)-OMEG@)/OMEG(K)
      IF(TST.GT.1.E-4) GO TO 210
  220 IF(KSWCH.GT.0) GO TO 230
      K=K+1
      IF(K.LT.4) GO TO 180
      KSNCH=1
  230 IF(K.EQ.2) GO TO 290
CCC
      ADJUST STARTING POSITIONS UNTIL THE TRAJECTORY K=2 PRODUCES THE
      MAXIMUM IONIZATION INTEGRAL.
      IF(PI(1).GT.PI(2)) GO TO 250
      IF(K.EQ.1) GO TO 240
```

```
IF(PI(3).GT.PI(2)) GO TO 270
  248 K=2
      GO TO 290
CC
      MAXINUM IS TO LEFT OF K=2. SHIFT LEFT ACCORDINGLY.
C
  258 K=1
      ISTART(2)=ISTART(1)
      JSTART(2)=JSTART(1)
      XSTART(2)=XSTART(1)
      YSTART(2)=YSTART(1)
      PI(2)=PI(1)
      KHTMX(2)=KHTMX(1)
      KMX=KNTMX(1)
      DO 260 KNT=1.KMX
      XPATH(KNT,2)=XPATH(KNT,1)
      YPATH(KNT,2)=YPATH(KNT,1)
  260 ET(KHT,2)=ET(KHT,1)
      I=ISTART(1)-2
      J=JSTART(1)-2
      IF(I.LT.0) GO TO 240
      GO TO 120
C
      MAXIMUM IS TO RIGHT OF K=2. SHIFT RIGHT ACCORDINGLY.
  270 K=3
      ISTART(2)=ISTART(3)
      JSTART(2)=JSTART(3)
      XSTART(2)=XSTART(3)
      YSTART(2)=YSTART(3)
      PI(2)=PI(3)
      KHTMX(2)=KHTMX(3)
      KNX=KNTNX(3)
      DO 280 KNT=1,KMX
      XPATH(KNT, 2)=XPATH(KNT, 3)
      YPATH(KNT,2)=YPATH(KNT,3)
  280 ET(KHT, 2)=ET(KHT, 3)
      I=ISTART(3)
      J=JSTART(3)
      IF(J.EQ.JMAX) GO TO 240
      GO TO 120
  290 EN1=EXP(PI(2))
      DEN=1.-OMEG(2)
      DN=ABS(DEN)
      IF(DN.LT.1.E-70) DEN=SIGN(1.E-70,DEN)
      EN2=1. /DEN
      WRITE(6,1030) VOLT, EM1, EM2
 1030 FORMAT(1H0,5X,'UOLT=',1PE10.2,3X,'M1=',1PE10.2,3X,'M2=',1PE10.2)
      IF(KOUTPT.GT.0) GO TO 90
      CALL OUTPUT
      GO TO 90
      END
```

SUPPLIES INITIAL ESTIMATE OF THE BREAKDOWN VOLTAGE USING AN EMPIRICAL FIT TO THE KENNEDY-O'BRIEN CURVES.

COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
&D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
&DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
&HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
COMMON/REAL/XWIDTH,YDEPTH,BRRIER,EGAP,TMPTR,ACCPTR,UBLTIN,UOLT,
&TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
COMMON/INTGR/IMAX,JMAX,IXWDTH,JYDPTH
COMMON/CNTRL/ITMAX,ITRMAX,CONURG,SIDLT
COMMON/HRMLZE/DNSNRM,PSINRM,DSTNRM,BLTZMN

C

RR=RAD
IF(RR.EQ.0) RR=0.1
AA=1./(18.+150.\*RR)
UNIT=1./(AA+3.75E-12\*DHSHRM\*\*0.6)
AA=2.303E4/(DHSHRM\*\*.3695)
BB=7.891E3/(DHSHRM\*\*.2968)
TT=TMPTR/300.-1.
UNIT=UNIT\*(AA\*TT\*TT+BB\*TT+1.)
RETURN
END

CCC

Y1=Y2 X2=X

```
00000000
```

USING UNNORMALIZED VARIABLES, CALCULATES THE TEMPERATURE-DEPENDENT BAND GAP, THE IONIZED ACCEPTOR DENSITY, AND THE BUILT-IN POTENTIAL BARRIER, ACCOUNTING FOR THE TEMPERATURE DEPENDENCE OF THE INTRINSIC DENSITY AND OF THE FERMI LEVEL.

```
COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      CONMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONVRG, SIDLT
      COMMON/HRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
      COMMON/SWICH/ NDOPE
C.
      T=TMPTR/3.E2
      BLTZMN=0.02585*T
      EGAP=1.165-7.242E-3*T-3.664E-2*T*T
      EIV=EGAP/2.E0-1.306E-2*T
      X=EIU
      KEY=1
      GO TO 170
C
      ADJUST X18X2 UNTIL Y18Y2 HAVE OPPOSITE SIGN
  100 X1=X
      Y1=Y
      DX=-EIV/2.E1
      IF(Y.LT.0.) DX=-DX
      X=X1+DX
      KEY=2
      GO TO 170
  110 X2=X
      Y2=Y
      IF(Y1*Y2.LE.0.) GO TO 140
  130 X1=X2
      Y1=Y2
      X=X2+DX
      GO TO 170
  140 KEY=3
C
      METHOD OF SECANTS
  150 IF(ABS(Y).LT.1.E-3) GO TO 180
      DEN=Y2-Y1
      X=(X1*Y2-X2*Y1)/DEN
      GO TO 170
  160 X1=X2
```

```
Y2=Y
G0 TO 150
CCC
       SUBROUTINE FOR EVALUATING Y
  170 EIF=X
      EFV=EIV-EIF
       EAF=4.38E-2-3.037E-8*ACCPTR**(1.0/3.0)-EFU
       BKGRND=ACCPTR/(1.0+(4.0+2.0/EXP(4.4E-2/BLTZMN))*EXP(EAF/BLTZMN))
       IF(NDOPE.GT.0) BKGRND=ACCPTR/(1.+2.*EXP(EAF/BLTZMN))
       TRNSIC=3.925E19*T*SQRT(T)*EXP(-EGAP/(2.*BLTZMN))
      BULKP=TRNSIC*EXP(EIF/BLTZMN)
       Y=(BULKP-BKGRND)/ACCPTR
      GO TO(100,110,160), KEY
CCCC
      CALCULATE THE BUILTIN POTENTIAL, THE ELECTRON DENSITY AT THE
      METAL-SILICON INTERFACE, AND THE BULK HOLE DENSITY.
  180 UBLTIN=BRRIER-EFU
      DHSHRM=BKGRND
      WRITE(6,1000)TMPTR, EGAP, EIU, EIF, EFU, TRNSIC, BKGRND, UBLTIN
 1000 FORMAT(2X,//,3X,'TMPTR',5X,'EGAP',7X,'EIV',7X,'EIF',7X,'EFV',
&6X,'TRNSIC',4X,'BKGRND',4X,'UBLTIN',//,1X,1P8E10.2,//)
      END
C
```

TRACKS WHICH 'BOX' OF THE LATTICE IS OCCUPIED BY THE MOVING CHARGE & SUPPLIES ITS INDICES (I,J) AND CORRECT VALUES FOR DLTX & DLTY WITH RESPECT TO THAT POINT. ALSO FLAGS AN EXIT OF THE CHARGE FROM THE REGION.

COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
&D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
&DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31),
COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
&HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
COMMON/REAL/XWIDTH,YDEPTH,BRRIER,EGAP,TMPTR,ACCPTR,VBLTIN,VOLT,
&TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
COMMON/INTGR/IMAX,JMAX,IXWDTH,JYDPTH
COMMON/CNTRL/ITMAX,ITRMAX,CONURG,SIDLT
COMMON/HRMLZE/DNSNRM,PSINRM,DSTNRM,BLTZMN

C

IF(DLTX.LT.0.) GO TO 100 IF(DLTX.GT.XDLT(I+1)) GO TO 110 GO TO 120

100 IF(I.EQ.1) GO TO 150 DLTX=XDLT(I)+DLTX I=I-1 IF(DLTX.LT.0.) GO TO 100 GO TO 120

110 IF(I.EQ.(IMAX-1)) GO TO 150 DLTX=DLTX-XDLT(I+1) I=I+1

IF(DLTX.GT.XDLT(I+1)) GO TO 110 120 IF(DLTY.LT.0.) GO TO 130 IF(DLTY.GT.YDLT(J)) GO TO 140

RETURN 130 IF(J.EQ.JMAX) GO TO 150 DLTY=YDLT(J+1)+DLTY J=J+1

IF(OLTY.LT.0.) GO TO 130

RETURN 140 IF(J.EQ.2) GO TO 150 DLTY=DLTY-YDLT(J) J=J-1

IFCOLTY.GT.YOLT(J)) GO TO 140

RETURN 150 KEXIT=1 RETURN END

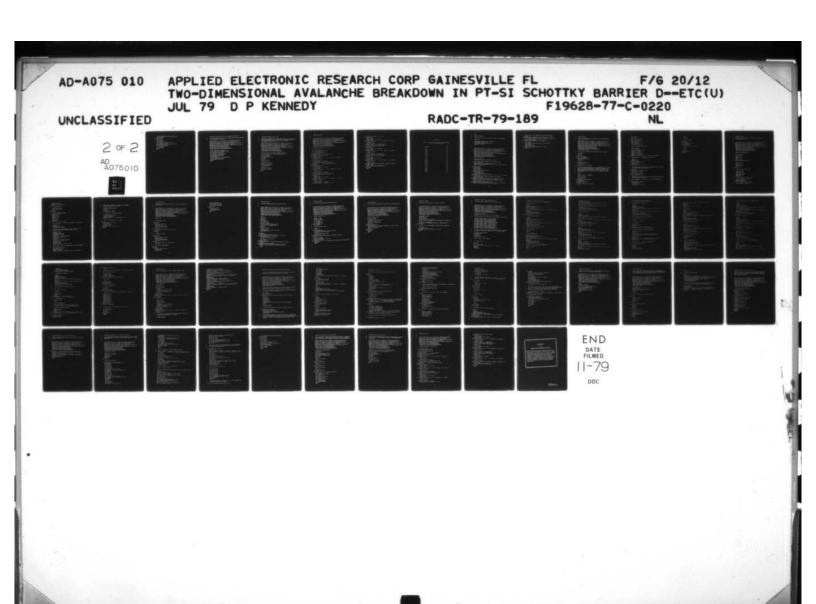
C

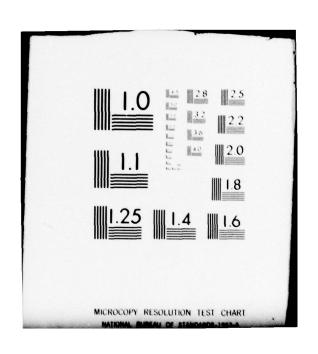
C	SUBRUUTINE EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET)
000000	APPLIES INTERPOLATION FOR THE X & Y COMPONENTS OF THE ELECTRIC FIELD AT LOCATION $(X,Y)$ .
CC	CONMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31), &D(31,31), E(31,31), F(31,31), H(31,31), Q(31,31), QAREA(31,31), &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31), CONMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31) &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31) CONMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT, &TRNSIC, QSS, XO, YO, RAD, XDELTA, YDELTA COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
c	COMMON/CNTRL/ITMAX,ITRMAX,CONURG,SIDLT COMMON/NRMLZE/DNSNRM,PSINRM,DSTNRM,BLTZMN
	100 EN=ESUBX(I,J)+DLTX*(ESUBX(I+1,J)-ESUBX(I,J))/XDLT(I+1) ES=ESUBX(I,J-1)+DLTX*(ESUBX(I+1,J-1)-ESUBX(I,J-1))/XDLT(I+1) EX=EN+DLTY*(ES-EN)/YDLT(J) EN=ESUBY(I,J)+DLTX*(ESUBY(I+1,J)-ESUBY(I,J))/XDLT(I+1) ES=ESUBY(I,J-1)+DLTX*(ESUBY(I+1,J-1)-ESUBY(I,J-1))/XDLT(I+1) EY=EN+DLTY*(ES-EN)/YDLT(J) ET=SQRT(EX*EX+EY*EY) RETURN
CC	END

```
SUBROUTINE TRAJEC(KNT, I, J, X, Y, OLTX, OLTY, ET, KEXIT)
00000000
      USES ADAMS-BASHFORTH-MOULTON PREDICTOR-CORRECTOR EQ'S TO TRACE
      HOLE TRAJECTORIES: FOLLOWING A FOURTH-ORDER RUNGE-KUTTA STARTING
      PROCEDURE.
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      CONNON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIOTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      CONMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      DIMENSION DX(7), DY(7)
C
      IF(KNT.GT.4) GO TO 100
      IF(KNT.GT.1) GO TO 90
      DLTA=0.005
      TOELT=OLTA/ET
      DO 80 K=1.7
      ON(K)=0.
   80 DY(K)=0.
CC
      RUNGE-KUTTA PROCEDURE
   90 CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      CALL EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET)
      DX1=EX*TOELT
      DY1=EY*TOELT
      XX=X+DX1/2.E0
      YY=Y+DY1/2.E0
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX2=EX*TOELT
      DY2=EY*TDELT
      XX=X+DX2/2.E0
      YY=Y+DY2/2.E0
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX3=EX*TDELT
      DY3=EY*TDELT
      XX=X+DX3
      YY=Y+DY3
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
```

```
CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX4=EX*TDELT
      DY4=EY*TDELT
      DX(KNT+3)=(DX1+2.E0*(DX2+DX3)+DX4)/6.E0
      DY(KNT+3)=(DY1+2.E0*(DY2+DY3)+DY4)/6.E0
      X=X+DX(KNT+3)
      Y=Y+DY(KNT+3)
      DLTX=X-XPOS(I)
      DLTY=Y-YPOS(J)
      CALL INDEX(I)JDLTX/DLTY/KEXIT)
      CALL EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET)
      DX(KHT+3)=EX*TDELT
      DY(KNT+3)=EY*TDELT
      KOBLE=3
      RETURN
CC
      PREDICTOR-CORRECTOR, USING THE PRESENT INTERVAL
C
  100 XPRDCT=(55.E0*DX(7)-59.E0*DX(6)+37.E0*DX(5)-9.E0*DX(4))/24.E0
      YPRDCT=(55.E0*DY(7)-59.E0*DY(6)+37.E0*DY(5)-9.E0*DY(4))/24.E0
      XX=X+XPROCT
      YY=Y+YPROCT
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      IF(KEXIT.GT.0) RETURN
      CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX1=EX*TDELT
      DY1=EY*TDELT
      XCRRCT=(9.E0*DX1+19.E0*DX(7)-5.E0*DX(6)+DX(5))/24.E0
      YCRRCT=(9.E0*DY1+19.E0*DY(7)-5.E0*DY(6)+DY(5))/24.E0
      DX2=ABS(XPRDCT-XCRRCT)
      DY2=ABS(YPRDCT-YCRRCT)
      DLT=AMAX1(DX2,DY2)
c
C
      HALVE THE INTERVAL IF DLT EXCEEDS DLTA
C
      IF(DLT.LT.DLTA) GO TO 110
c
      PARABOLIC INTERPOLATION COEFFICIENTS FOR THE HALF INTERVAL VALUES
      KDBLE=3
      TOELT=TOELT/2.EU
      AA=(DX(7)-2.E0*DX(6)+DX(5))/(8.E0*TDELT*TDELT)
      BB=(DX(7)-DX(5))/(4.E0*TDELT)
      AAA=(DX(6)-2.E0*DX(5)+DX(4))/(8.E0*TDELT*TDELT)
      BBB=(DX(6)-DX(4))/(4.E0*TDELT)
      OX(1)=OX(4)/2.E0
      DX(3)=DX(5)/2.E0
      DX(5)=DX(6)/2.E0
      DX(2)=(TDELT*(AAA*TDELT-BBB)+DX(3))/2.E0
      DX(4)=(TDELT*(AA*TDELT-BB)+DX(5))/2.E0
      DX(6)=(TDELT*(AA*TDELT+BB)+DX(5))/2.E0
      DX(7)=DX(7)/2.E0
      AA=(DY(7)-2,E0*DY(6)+DY(5))/(8.E0*TOELT*TDELT)
      BB=(DY(7)-DY(5))/(4.E0*TDELT)
```

```
AAA=(DY(6)-2.E0*DY(5)+DY(4))/(8.E0*TDELT*TDELT)
      BBB=(DY(6)-DY(4))/(4.E9*TDELT)
      DY(1)=DY(4)/2.E0
      DY(3)=DY(5)/2.E0
      DY(5)=DY(6)/2.E0
      DY(2)=(TDELT*(AAA*TDELT-BBB)+DY(3))/2.E0
      DY(4)=(TDELT*(AA*TDELT-BB)+DY(5))/2.E0
      DY(6)=(TDELT*(AA*TDELT+BB)+DY(5))/2.E0
      DY(7)=DY(7)/2.E0
      GO TO 100
      TENTATIVELY DOUBLE THE INTERVALIBUT ONLY IF 3 STEPS HAVE BEEN
CC
      TAKEN SINCE THE LAST DOUBLING OR HALVING, AND ONLY IF DLT
      IS LESS THAN ONE HALF OF DLTA
  110 IF(KDBLE.GT.0) GO TO 120
      DLT=DLT#2.0
      IF(OLT.GT.DLTA) GO TO 120
      XPRDT=(55.E0*DX(7)-59.E0*DX(5)+37.E0*DX(3)-9.E0*DX(1))/12.E0
      YPRDT=(55.E0*DY(7)-59.E0*DY(5)+37.E0*DY(3)-9.E0*DY(1))/42.E0
      XX=X+XPRDT
      YY=Y+YPROT
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      IF(KEXIT.GT.0) GO TO 120
      CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX1=EX*TDELT
      DY1=EY*TDELT
      XCRRT=(9.E0*DX1+19.E0*DX(7)-5.E0*DX(5)+DX(3))/12.E0
      YCRRT=(9.E0*DY1+19.E0*DY(7)~5.E0*DY(5)+DY(3))/12.E0
      DX2=ABS(XPRDT-XCRRT)
      DY2=ABS(YPRDT-YCRRT)
      DLT=AMAX1(DX2,DY2)
      IF(DLT.GT.DLTA) GO TO 120
      DOUBLE INTERVAL IS OK, SO DO IT
      DX(7)=DX(7)*2.E0
      DX(6)=DX(5)*2.E0
      DX(5)=DX(3)*2.E0
      DX(4)=DX(1)*2.E0
      DY(7)=DY(7)*2.E0
      DY(6)=DY(5)*2.E0
      DY(5)=DY(3)*2.E0
      DY(4)=DY(1)*2.E0
      X=X+(19.E0*XPRDT+251.E0*XCRRT)/270.E0
      Y=Y+(19.E0*YPRDT+251.E0*YCRRT)/270.E0
      TDELT=2.E0*TDELT
      KOBLE=3
      GO TO 130
CCC
      NO DOUBLING OCCURRED. COMPUTE NEW X & Y. SHIFT INCREMENTS LEFT
      & UPDATE THE MOST RECENT INCREMENT.
  120 X=X+<19.E0*XPRDCT+251.E0*XCRRCT>/270.E0
```





```
Y=Y+(19.E0*YPROCT+251.E0*YCRRCT)/270.E0
    KOBLE=KOBLE-1
130 DO 140 K=1.6
    DX(K)=DX(K+1)
140 DY(K)=DY(K+1)
    DLTX=X-XPOS(I)
    DLTY=Y-YPOS(J)
    CALL INDEX(I, J, DLTX, DLTY, KEXIT)
    IF(KEXIT.GT.0) RETURN
   CALL EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET)
   ETT=ET*PSINRM/DSTNRM
    IF(ETT.LT.2.E4) KEXIT=1
   DX(7)=EX*TDELT
   DY(7)=EY*TOELT
   RETURN
   END
```

SUBROUTINE JNTGRL(DX,DY,ET1,ET2,PI,RR,OMEG,ALPHN,ALPHP)

CCCC

USES TRAPEZOIDAL RULE FOR THE TWO-CARRIER MULTIPLICATION INTEGRAL. (USES DIMENSIONED VARIABLES.)

COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
&D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
&DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31),
COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
&HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31),
COMMON/REAL/XWIDTH,YDEPTH,BRRIER,EGAP,TMPTR,ACCPTR,VBLTIN,VOLT,
&TRNSIC,QSS,X0,Y0,RAO,XDELTA,YDELTA
COMMON/INTGR/INAX,JMAX,IXWDTH,JYDPTH
COMMON/CNTRL/ITMAX,ITRMAX,CONVRG,SIDLT
COMMON/HRMLZE/DNSNRM,PSINRM,DSTNRM,BLTZMN

C

- 5

DS=SQRT(DX\*DX+DY\*DY)\*DSTNRM
ET=(ET1+(ET2-ET1)/4.)\*PSINRM/DSTNRM
CALL TWNSND(ET,ALPHN,ALPHP)
RR=RR+(ALPHN-ALPHP)\*DS/2.
ET=((ET1+ET2)/2.)\*PSINRM/DSTNRM
CALL TWNSND(ET,ALPHN,ALPHP)
OMEG=OMEG+ALPHP\*EXP(RR)\*DS
PI=PI+ALPHN\*DS
ET=(ET1+3.\*(ET2-ET1)/4.)\*PSINRM/DSTNRM
CALL TWNSND(ET,ALPHN,ALPHP)
RR=RR+(ALPHN-ALPHP)\*DS/2.
RETURN
END

000000

CALCULATES THE TOWNSEND IONIZATION COEFFICIENTS FOR ELECTRONS AND HOLES USING CRONELL & SZE,S EMPIRICAL FIT FOR BARAFF,S CURVES. USES UNNORMALIZED VARIABLES. (SEE S.M.SZE, PHYSICS OF SEMICONDUCTOR DEVICES, PP 61-65.)

COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
&D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
&DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,3')
COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
&HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
COMMON/REAL/XWIDTH,YDEPTH,BRRIER,EGAP,TMPTR,ACCPTR,UBLTIN,UOLT,
&TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
COMMON/INTGR/IMAX,JMAX,IXWDTH,JYDPTH
COMMON/CNTRL/ITMAX,ITRMAX,CONURG,SIDLT
COMMON/HRMLZE/DNSNRM,PSINRM,DSTNRM,BLTZMN

C

EXPNT(R2,R1,X2,X1)=(11.5\*R2-1.17\*R1+3.9E-4)\*X2 + &(46. \*R2-11.9\*R1+1.75E-2)\*X1-(757. \*R2-75.5\*R1+1.91) TANH(X) = (EXP(X) - EXP(-X))/(EXP(X) + EXP(-X))XX=3.15E-2/BLTZMN EP=6.3E-2\*TANH(XX) ELMBDA=76.0E-8\*EP/6.3E-2 EI=1.5\*EGAP R1=EP/EI R2=R1\*R1 X1=EI/(ET\*ELMBDA) X2=X1\*X1 XN=EXPNT(R2,R1,X2,X1) IF(XN.LT.-80.) XN=-80. ALPHN=EXP(XN)/ELMBDA ELMBDA=50.0E-8\*EP/6.3E-2 X1=EI/(ET\*ELMBDA) X2=X1\*X1 XH=EXPNT(R2,R1,X2,X1) IF(XN.LT.-80.) XN=-80. ALPHP=EXP(XH)/ELMBDA RETURN END

140 SCRTCH(I)=HDENS(I,J)\*DNSNRM

WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)

WRITE(6,1040)(SCRTCH(I),I=11,IMAX)

150 CONTINUE

WRITE(6,1000)

WRITE(6,1000)

1100 FORMAT(1H0,5X,'J',9X,'Y(J)',15X,'EDENS(I,J),I=1,IMAX',//)

DO 154 JJ=1,JMAX

J=JMAX+1-JJ

DO 152 L=1,IMAX

152 SCRTCH(I)=EDENS(I,J)\*DNSNRM

WRITE(6,1030)J,Y(J),(SCRTCH(I),I=1,10)

```
WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
154 CONTINUE
    NRITE(6,1000)
    MRITE(6, 1010)(X(I), I=1, IMAX)
    WRITE(6,1070)
1070 FORMAT(1H0,5%,'J',9%,'Y(J)',15%,'ESUBX(I,J),I=1,IMAX',//)
    DO 170 JJ=1, JMAX
     J=JMAX+1-JJ
    DO 160 I=1. IMAX
 160 SCRTCH(I)=ESUBX(I,J)*PSINRM/OSTNRM
    WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
    WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
 170 CONTINUE
    WRITE(6, 1000)
    WRITE(6,1010)(X(I),I=1,IMAX)
    WRITE(6, 1080)
1080 FORMAT(1H0,5%,'J',9%,'Y(J)',15%,'ESUBY(I,J),I=1,IMAX',//)
    DO 190 JJ=1, JMAX
     J=JMAX+1-JJ
    DO 180 I=1 IMAX
 180 SCRTCH(I)=ESUBY(I,J)*PSINRM/DSTNRM
    WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
    WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
190 CONTINUE
    WRITE(6, 1000)
    WRITE(6,1010)(X(I),I=1,IMAX)
    WRITE(6, 1090)
1090 FORMAT(1H0,5%,'J',9%,'Y(J)',15%,'ETOTAL(I,J),I=1,IMAX',//)
    DO 210 JJ=1, JMAX
    J=JMAX+1-JJ
    DO 200 I=1, IMAX
200 SCRTCH(I)=SQRT(ESUBX(I,J)*ESUBX(I,J)+ESUBY(I,J)*ESUBY(I,J))*
   &PSINRM/DSTNRM
    WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
    WRITE(6,1040)(SCRTCH(I),I=11,INAX)
210 CONTINUE
    RETURN
    END
```

Appendix B

## Computer Program Listing For Calculation Avalanche Breakdown in a Pt-Si Schottky Barrier Diode

Subroutine	Page
MAIN	104
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```
cccccc
      MAIN
      EXECUTIVE PROGRAM
      INITIALIZE ALL ARRAYS TO ZERO WITH A BLOCK DATA SUBPROGRAM
      BLOCK DATA
C
      COMMON/ARRAYS/ADUMNY(12493), IDUMNY(961)
      COMMON/COEFF/COUMMY(4931)
      DATA ADUMNY/12493*0./, IDUMNY/961*0/
      DATA CDUMMY/4931*0.E0/
      END
C
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWOTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
      COMMON/SWICH/NDOPE
C
      DIMENSION TITLE (54)
      DIMENSION XPATH(100,3), YPATH(100,3), ET(100,3)
C
      NAMELIST/GEOM/XWIDTH, YDEPTH, IMAX, JMAX, NXWDTH, NYDPTH,
     &XDELTA, YDELTA, RAD
      NAMELIST/PRMTRS/ACCPTR,BRRIER,QSS,TMPTR
      NAMELIST/CONTRL/ITMAX, ITRMAX, CONURG, SIDLT, AUDLT, ULTDLT, KNTNAX
      NAMELIST/SWITCH/NDOPE
  100 READ(5, GEOM)
      READ(5, PRMTRS)
      READ(5, CONTRL)
      READ(5, SWITCH)
      READ(5,1000) (TITLE(I), I=1,54)
 1000 FORMAT(18A4/18A4/18A4)
      IXWDTH=NXWDTH
      JYDPTH=JMAX-NYDPTH+1
      WRITE(6, 1010)(TITLE(I), I=1,54)
 1010 FORMAT(1H1,60X,/,30X,18A4,/,30X,18A4,/,30X,18A4,//,5X,'SUMMARY
     &OF INPUT DATA : ', //)
      WRITE(6,1020) XWIDTH, YDEPTH, IMAX, JMAX, NXWDTH, NYDPTH,
     &XDELTA, YDELTA, RAD
 1020 FORMAT(1H0,5%, 'NAMELIST/GEOM/ XWIDTH=',1PE10.2,2%,'YDEPTH=',
     &1PE10.2.2X,'IMAX=',I3.2X,'JMAX=',I3.2X,'NXNDTH=',I3.2X,
&'NYDPTH=',I3.2X,'XDELTA=',1PE10.2,/,6X,'YDELTA=',1PE10.2,2X,
     &'RAD=',1PE10.2,/)
      WRITE(6,1030)ACCPTR, BRRIER, QSS, TMPTR
 1030 FORMAT(1H0,5%, 'NAMELIST/PRMTRS/ ACCPTR=',1PE10.2,2%, 'BRRIER=',
     &1PE10.2,2X,'QSS=',1PE10.2,2X,'TMPTR=',1PE10.2)
```

```
WRITE(6,1040) ITMAX, ITRMAX, CONVRG, SIDLT, AUDLT, ULTDLT, &KHTMAX

1040 FORMAT(1H0,5%, 'NAMELIST/CONTRL/ ITMAX=',13,2%, 'ITRMAX=', &13,2%, 'CONVRG=',1PE10.2,2%, 'SIDLT=',1PE10.2,2%, 'KNTMAX=',14,/)

WRITE (6,1060) NDOPE

1060 FORMAT(1H0,5%, 'NAMELIST/SWITCH/ NDOPE=',12,/)

C

CALL INTGR1

CALL AULNCH(ULTDLT, AUDLT, XPATH, YPATH, ET, KNTMAX)

CALL OUTPUT

UOLT=PSIHRM-UBLTIN

WRITE(6,1050) UOLT

1050 FORMAT(1H0,5%, 'BREAKDOWN UOLTAGE=',1PE10.2)

GO TO 100

END

C

C
```

```
SUBROUTINE GRID
      SETS UP THE GRADED LATTICE & COMPUTES THE FINITE-DIFFERENCE
      COEFFICIENTS FOR PSI.
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/CDEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XNIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC, QSS, XO, YO, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDFTH
      COMMON/CNTRL/ITMAX,ITRMAX,CONURG,SIDLT
      COMMON/NRMLZE/ONSHRM, PSINRM, DSTNRM, BLTZMN
      COMMON/RSCALE/ RSFCTR
CCC
      FIRST TREAT THE CORNER REGION BOUNDED BY XWIDTH & YDEPTH.
      INX=IXNDTH-1
      X=XDELTA
      KEY=1
      GO TO 200
  100 XDLT(2)=XWIDTH*DLT
      DO 110 I=3. INNOTH
  110 XDLT(I)=XDLT(I-1)*XDELTA
      INX=JMAX-JYDPTH
      X=YDELTA
      KEY=2
      GO TO 200
  120 YOLT(JMAX)=YDEPTH*DLT
      00 130 J=2, IMX
      L-1+XAML=LL
  130 YDLT(JJ)=YDLT(JJ+1)*YDELTA
CCCCCCC
      NEXT TREAT THE REGION EXTERNAL TO THE CORNER REGION. THIS REGION
      EXTENDS 1.25 DEPLETION WIDTHS TO THE RIGHT OF X=XWIDTH, AND
      BELON Y=YDEPTH. USE THE METHOD OF SECANTS TO DETERMINE THE
      MULTIPLIERS ANALOGOUS TO XDELTA & YDELTA LEADING TO A SMOOTH
      TRANSITION IN THE LATTICE SPACINGS AT THE INTERFACE OF THE
      THO REGIONS.
      KEY=3
      KED=1
      CC=XDLT(IXWDTH)/(1.25*RSFCTR)
      X1 = 1
      IMX=IMAX-IXWDTH
      Y1=(1./IMX-CC)/CC
      GO TO 230
  140 XDLT(IMAX)=1.25*RSFCTR*DLT
      00 150 I=2, IMX
      II=IMAX+1-I
  150 XDLT(II)=XDLT(II+1)*X
      KED=2
      CC=YDLT(JYDPTH+1)/(1.25*RSFCTR)
      X1 = 1.
```

```
INX=JYDFTH-1
      Y1=(1./IMX-CC)/CC
      GO TO 230
  160 YOLT(2)=1.25*RSFCTR*OLT
      DO 170 J=3, JYDPTH
  170 YOLT(J)=YOLT(J-1)*X
      XDLT(1)=XDLT(2)
      XDLT(IMAX+1)=XDLT(IMAX)
      YDLT(1)=YDLT(2)
      YDLT(JMAX+1)=YDLT(JMAX)
CCC
      FINITE-DIFFERENCE COEFFICIENTS
      DO 175 I=1, IMAX
      DO 175 J=1, JMAX
      NAU=(XDLT(I)+XDLT(I+1))/2
      YAU=(YDLT(J)+YDLT(J+1))/2.
      QAREA(I, J)=XAU*YAU
      HSTH(I,J)=XAU/YDLT(J)
      HWEST(I,J)=YAU/XDLT(I)
      HEAST(I, J)=YAU/XOLT(I+1)
      HNRTH(I,J)=XAU/YDLT(J+1)
  000
      TABULATE THE X & Y COORDINATES OF THE LATTICE.
      XPOS(1)=0
      YPOS(JMAX)=0
      DO 180 I=2, IMAX
  180 XPOS(I)=XPOS(I-1)+XDLT(I)
      DO 190 J=2, JMAX
      JJ=JMAX+1-J
  190 YPOS(JJ)=YPOS(JJ+1)+YDLT(JJ+1)
      GO TO 270
CC
      INSTRUCTIONS 200 THROUGH 220 ARE A SUBPROGRAM FOR CALCULATING
      THE WIDEST NORMALIZED INCREMENT OLT.
  200 EPSLON=1.-X
      IF(EPSLON.LT.1.E-3) GO TO 210
      DLT=(1.-X)/(1.-X**IMX)
      GO TO 220
  210 DLT=1.-(INX-1)*EPSLON/2.
      DLT=1./(IMX*DLT)
  220 GO TO(100,120,250),KEY
C
      INSTRUCTIONS 230 THROUGH 260 ARE A SUBPROGRAM FOR FINDING DLT
CCCC
      USING THE METHOD OF SECANTS.
      FIRST INCREMENT X1 & X2 UNTIL Y1 & Y2 HAUE OPPOSITE SIGNS.
  230 X2=X1-0.02
      Y2=(1,-X2)/(1,-X2**INX)
      Y2=Y2*X2**(IMX-1)
      Y2=(Y2-CC)/CC
      IF(Y1*Y2.LE.0.) GO TO 240
```

```
X1=X2

Y1=Y2

GO TO 230

C METHOD OF SECANTS

C 240 DEN=Y2-Y1

X=(X1*Y2-X2*Y1)/DEN

GO TO 200

250 Y=DLT*X**(INX-1)

Y=(Y-CC)/CC

IF(ABS(Y).LT.0.01) GO TO 260

X1=X2

Y1=Y2

X2=X

Y2=Y

GO TO 240

260 GO TO(140,160),KED

270 RETURN

END
```

```
SUBROUTINE BORDER
C
ccccc
      ASSIGNS BOUNDARY CONDITIONS BY MODIFYING THE FINITE-
      DIFFERENCE COEFFICIENTS
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/INAX, JMAX, IXNOTH, JYDFTH
       COMMON/CHIRL/ITMAX, ITRMAX, CONURG, SIDLT
      CONMON/NRMLZE/ONSNRM, PSINRM, DSTNRM, BLTZMN
C
       CIRCLE(X,Y,R)=X*X+Y*Y-R*R
      POINT(Z,R)=SQRT(R*R-Z*Z)
C
      DO 98 I=1. INAX
      DO 90 J=1, JMAX
      PSI(I, J)=0
      HDENS(I,J)=0
      ESUBX(I, J)=0.
      ESUBY(I, J)=0.
   90 IDENT(1,J)=0
C
       THE LOWER BORDER, WHERE PSI=0
      DO 100 I=1, IMAX
      HSTH( I, 1 )=0.
      HNEST(I,1)=0.
      HCHTR( I, 1 )=1 . E@
      HEAST(1,1)=0.
      HNRTH(I,1)=0.
  100 Q(1,1)=0.
000
       THE RIGHT BORDER, WHERE PSI=0.
      .00 118 J=1, JMAX
      HSTHCIMAX, J)=0.
      HWEST(IMAX, J)=0.
      HCNTR(IMAX, J)=1.E0
      HEAST(IMAX, J)=0.
       HNRTH(IMAX,J)=0.
  118 QCIMAX, J)=0.
CCC
       THE UPPER BURDER, WHERE DPSI/DY=0.
      DO 120 I=IXWDTH, IMAX
       HNRTH(I,JMAX)=0
  120 HSTH(I, JMAX)=2.E0*HSTH(I, JMAX)
CCC
      THE LEFT BORDER, WHERE DPSI/DX=0.
```

```
DO 130 J=1.JYDPTH
      HWEST(1, J)=0.
  130 HEAST(1, J)=2.E0*HEAST(1, J)
CCC
      THE CORNER REGION
      X0=XPOS(IXWDTH)~RAD
      Y0=YPOS(JYDPTH)-RAD
      I=1
  140 J=JMAX+1
  150 J=J-1
      IF (J.LT. JYDPTH)GO TO 180
      IF (XPOS(I).GT.X0)GO TO 170
  160 HSTH(I,J)=0.
      HWEST(I,J)=0.
      HCMTR(I,J)=1.E0
      HEAST(I,J)=0.
      HNRTH(I,J)=0.
      Q(I,J)=1.0
      IDENT(I,J)=-1
      GO TO 150
  170 IF(YPOS(J).LE.Y0)GO TO 160
C
      TEST TO DETERMINE IF THE POINT IS EXTERNAL TO THE CIRCLE.
C
      XP=XPOS(I)-X0
      YP=YPOS(J)-Y0
      TSTP=CIRCLE(XP, YP, RAD)
      IF(TSTP.LE.0.)GO TO 160
      FIND THE WEST & NORTH DISTANCES TO THE BOUNDARY.
                                                          FIRST
      DETERMINE WHICH POINTS ARE ALSO EXTERNAL, IF ANY.
      XW=XPOS(I-1)-X0
      YN=YPOS(J+1)-Y0
      TSTN=CIRCLE(XW, YP, RAD)
      TSTN=CIRCLE(XP, YN, RAD)
      XW=XPOS(I-1)
      IF(ISTW.LT.0.)XW=X0+POINT(YP,RAD)
      IF(TSTW.LT.0.) IDENT(I,J)=1
      XN=XPDS(1)-XW
      YN=YPOS(J+1)
      IF(TSTN.LT.0.)YN=Y0+P0INT(XP,RAD)
      IF(TSTN.LT.0.) IDENT(I,J)=1
      YN=YPOS(J)-YN
      XWW=XDLT(I)/100.
      YNN=YDLT(J)/100.
      IF(XW.LT.XWW.OR.YN.LT.YNN) GO TO 160
      MODIFY HWEST & HNRTH, TO ACCOUNT FOR THE CIRCULAR BOUNDARY.
      XAU=(XDLT(I+1)+XW)/2.E0
      YAV=(YN+YDLT(J))/2.E0
      HWEST(I,J)=YAU/XW
      HHRTH(I,J)=XAU/YN
      HCNTR(I,J)=-(HSTH(I,J)+HWEST(I,J)+HEAST(I,J)+HNRTH(I,J))
```

```
CCCC
      MODIFY GAREA TO ACCOUNT FOR THE PORTION (ASSUMED A
      TRIANGLE) ECLIPSED BY THE CIRCLE.
      X1=XPOS(I)-XDLT(I)/2.E0
      Y1=YPOS(J)-YDLT(J+1)/2.E0
      XP=X1-X0
      YP=Y1-Y0
      TSTP=CIRCLE(XP, YP, RAD)
000
      IF (TSTP.GE.0.) NO AREA IS ECLIPSED.
      IFCTSTP.GE.O. DGO TO 150
      Y2=P0INT(XP,RAD)+Y0
      X3=POINT(YP,RAD)+X0
      QAREA(I, J)=QAREA(I, J)-(Y2-Y1)*(X3-X1)/2.E0
      GO TO 150
CCC
      INDEX I & CONTINUE UNTIL I.GT. IXNOTH.
  180 I=I+1
      IF(I.LE.IXWDTH) GO TO 140
      IMAXX=IMAX-1
      DO 190 1=1. IMAXX
      DO 190 J=2, JMAX
  198 IF(IDENT(I, J).LT.0) PSI(I, J)=1.0
      RETURN
      END
CC
```

```
SUBROUTINE NITIAL
ccccccc
      SUPPLIES INITIAL ESTIMATE FOR PSI(I,J), USING THE DEPLETION
      APPROXIMATION
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/CDEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, WOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/INAX, JNAX, IXNOTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      RD=RAD+1.0
      I=1
CC
      THE HORIZONTAL SHEATH
  100 J=JYDPTH
  110 J=J-1
      IF(J.EQ.1) GO TO 120
      RR=YPOS(J)-Y0
      IF(RR.GE.RD) GO TO 120
      PSI(I,J)=(RD-RR)*(RD-RR)
      GO TO 110
  120 I=I+1
      IF(I.EQ.IMAX.OR.XPOS(I).GT.X0) GO TO 130
      GO TO 100
  130 IM=I-1
      J=JMAX
CCC
      THE VERTICAL SHEATH
  140 I=IXWDTH
  150 I=I+1
      IF(I.EQ.IMAX) GO TO 160
      RR=XPOS(I)-X0
      IF(RR.GE.RD) GO TO 160
      PSI(I,J)=(RD-RR)*(RD-RR)
      GO TO 150
  160 J=J-1
      IF(J.EQ.1.OR.YPOS(J).GT.Y0) GO TO 170
      GO TO 140
CCC
      THE CIRCULAR CORNER SHEATH
  170 I=IM
  180 I=I+1
      IF(I.EQ.IMAX) GO TO 190
      XP=XPOS(I)-X0
      YP=YPOS(J)-Y0
```

```
RR=SQRT(XP*XP+YP*YP)
IF(RR.LE.RAD) GO TO 180
IF(RR.GE.RD) GO TO 190
PSI(I,J)=(RD-RR)*(RD-RR)
GO TO 180
190 J=J-1
IF(J.LE.1) RETURN
YP=YPOS(J)-Y0
IF(YP.GE.RD) RETURN
GO TO 170
END
C
C
```

```
SUBROUTINE GRELAX
CCCCCC
      IMPLEMENTS GUMMEL'S RELAXATION ALGORITHM FOR PSI
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      OMEGA=1.6
      IT=1
      INAXX=INAX-1
  100 DLTMX=0
      CALL DHSITY
      CALL POISSN
      DO 110 I=1, IMAXX
      DO 110 J=2, JMAX
      DLTHX=AMAX1(ABS(DELTA(I,J)), DLTMX)
      PSI(I,J)=PSI(I,J)+OMEGA*DELTA(I,J)
      IF(PSI(I,J),LT,\theta,) PSI(I,J)=\theta.
  110 CONTINUE
      DMX=0.
      DO 500 I=1, IMAXX
      00 500 J=2, JMAX
      IF(ABS(DELTA(I,J)).LE.DMX) GO TO 500
      DMX=ABS(DELTA(I,J))
      II=I
      JJ=J
  500 CONTINUE
      WRITE(6,5000) DELTA(II,JJ),II,JJ
 5000 FORMAT(1H0,5%, 'MAX DELTA IN GRELAX IS',1PE11.3,1%,
     &'AT COORDINATE (',12,',',12,')')
      IF(DLTMX.LE.CONURG) GO TO 120
      IT=IT+1
      IF(IT.GT.ITMAX) GO TO 130
      GO TO 100
  120 WRITE(6,1000) IT
 1000 FORMAT(1H0,5X,15,'
                           ITERATIONS WERE REQUIRED IN GRELAX', ///)
      RETURN
  130 WRITE(6,1010) DLTMX, CONURG
1010 FORMAT(1H0,5%, 'MAXIMUM ITERATIONS WERE EXCEEDED IN
     &GRELAX.
                DLTMX=',1PE10.2,' CONURG=',1PE10.2,//)
      STOP
      END
```

```
SUBROUTINE POISSN
CCCCC
      SOLVES POISSONS EQUATION USING STONES METHOD.
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31.31),E(31.31),F(31.31),H(31.31),Q(31.31),QAREA(31.31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
      COMMON/CNTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
      DIMENZR: TZRGEW(31,31)
C
      DO 100 I=1, IMAX
      DO 100 J=1, JMAX
      PSINEW(I,J)=PSI(I,J)
      B(I,J)=HSTH(I,J)
      D(I,J)=HWEST(I,J)
      E(I,J)=HCNTR(I,J)
      F(I,J)=HEAST(I,J)
  100 H(I,J)=HNRTH(I,J)
      CALL CHARGE
CCC
      ITERATIVE STONE'S METHOD
      ISTONE=0
      ITR=1
  110 ISTONE=ISTONE+1
      CALL STONE(ISTONE, IMAX, JMAX, RESID, PSINEW)
      IF(RESID.LE.SIDLT) GO TO 120
      ITR=ITR+1
      IF(ITR.LE.ITRMAX) GO TO 110
      WRITE(6,1000)
 1000 FORMAT(1H0,1X, 'MAXIMUM ITERATIONS EXCEEDED IN POISSN',/)
      STOP
  120 DO 130 I≈1, IMAX
      DO 130 J≈1, JMAX
  130 DELTA(I,J)=PSINEW(I,J)-PSI(I,J)
      WRITE(6,5000) ITR
 5000 FORMAT(2X,//,2X,I5,1X,'ITERATIONS WERE REQUIRED WITH STONES METHOD
     &IN POISSN')
      RETURN
      END
```

130 CONTINUE RETURN END

116

```
SUBROUTINE CHARGE
00000
      CALCULATES THE CHARGE TERMS IN GUMMELS ALGORITHM
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMON/INTGR/IMAX, JMAX, IXNDTH, JYDPTH
      COMMON/CHTRL/ITMAX,ITRMAX,CONURG,SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
C
      ALPHA=PSINRM/BLTZMN
      IMAXX=IMAX-1
      00 100 I=1.IMAXX
00 100 J=2.JMAX
      IF(IDENT(I,J).LT.0) GO TO 100
      Q(I,J)=1.+EDENS(I,J)-HDENS(I,J)-ALPHA*(EDENS(I,J)+HDENS(I,J))*
     &PSI(I,J)
      Q(I,J)=2.*Q(I,J)*QAREA(I,J)
      E(I,J)=E(I,J)-2.*(EDENS(I,J)+HDENS(I,J))*ALPHA*QAREA(I,J)
  100 CONTINUE
CCC
      MODIFY Q AT THE UPPER BORDER TO INCLUDE SURFACE CHARGE QSS.
      II=IXNDTH+1
      DO 110 I=II. IMAX
  110 Q(I,JMAX)=Q(I,JMAX)-QSS*(XDLT(I)+XDLT(I+1))
      RETURN
      END
CC
```

```
SUBROUTINE STONE(ISTONE, JMAX, KMAX, RESID, T)
CCC
      IMPLEMENTS STONE'S METHOD FOR MATRIX FACTORIZATION.
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31)
      COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRNSIC.QSS.X0,Y0.RAD,XDELTA,YDELTA
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      CONMON/HRMLZE/DHSHRM, PSINRM, DSTHRM, BLTZMH
C
      DINENSION T(JMAX, KMAX)
      DIMENSION EE(31,31), FF(31,31), U(31,31), ALPHA(18)
C
      DEFINE FREQUENTLY USED FUNCTIONS. (N FOR FORWARD KIR FOR REVERSE).
      BN(BDUMMY, EDUMMY)=BDUMMY/(1.E0+ALPH*EDUMMY)
      CHCODUMMY, FOUMMY)=DOUMMY/(1.E0+ALPH*FOUMMY)
      DN1(EDUMMY,FDUMMY)=88*(ALPH*EDUMMY-FDUMMY)
      DN2(FDUMMY, EDUMMY)=CC*(ALPH*FDUMMY-EDUMMY)
      EN(FDUMMY,EDUMMY)=(FDUMMY-ALPH*BB*EDUMMY)/DD
      FN(HDUMMY, FDUMMY)=(HDUMMY-ALPH*CC*FDUMMY)/DD
      BR(HDUMMY, EDUMMY)=HDUMMY/(1, E0+ALPH*EDUMMY)
      CR(DDUMMY,FDUMMY)=DDUMMY/(1.E0+ALPH*FDUMMY)
      DR1(EDUMNY,FDUMNY)=BB*(ALPH*EDUMNY-FDUMNY)
      DR2(FDUMMY,EDUMMY)=CC*(ALPH*FDUMMY-EDUMMY)
      ER(FDUMMY, EDUMMY)=(FDUMMY-ALPH*BB*EDUMMY)/DD
      FR(BDUMMY)FDUMMY)=(BDUMMY-ALPH*CC*FDUMMY)/DD
cccc
      ISTONE FLAGS WHICH ALPHA TO USE AND WHETHER FORWARD (ISTONE ODD)
      OR REVERSE (ISTONE EVEN) INDEXING OF K IS TO BE IMPLEMENTED.
      IF(ISTONE.GT.18) ISTONE=1
      ALPH=ALPHA(ISTONE)
      JMAXX=JMAX-1
      KMAXX=KMAX-1
      J=2*(ISTONE/2)
      IF(J.EQ.ISTONE) GO TO 170
cccccc
      ISTONE IS ODD. INDEX K FORWARD
      THE CORNER POINT (1,1)
      DD = E(1, 1)
      EE(1,1)=F(1,1)/DD
      FF(1,1)=H(1,1)/DD
      R=Q(1,1)-(E(1,1)*T(1,1)+F(1,1)*T(2,1)+H(1,1)*T(1,2))
      RR=ABS(R)
      RESID=RR
```

U(1,1)=R/DD

```
IF(A8S(U(1,1)).LT.1.E-7) U(1,1)=0.
CCC
                  THE RON K=1. EXCLUDING THE RIGHT CORNER POINT.
                  00 100 J=2, JMAXX
                  JP=J+1
                  JH= J-1
                  CC=CN(D(J,1),FF(JN,1))
                  DD=E(J,1)+DN2(FF(JN,1),EE(JN,1))
                  EE(J,1)=F(J,1)/00
                  FF(J,1)=FN(H(J,1),FF(JN,1))
                  R = Q(J_0 + 1) + (D(J_0 + 1) + T(J_0 + 1) 
                &T(J, 2))
                  RR=ABS(R)
                  IF (RR.GT.RESID) RESID=RR
                  U(J,1)=(R-CC*U(JN,1))/DD
       100 IF(ABS(U(J,1)).LT.1.E-7) U(J,1)=0.
 CCC
                  THE CORNER POINT (JMAX, 1)
                  J=JMAX
                  XXAML=NL
                  CC=CN(D(J,1),FF(JN,1))
                  DD=E(J,1)+DN2(FF(JN,1),EE(JN,1))
                  EE(J,1)=0.
                  FF(J,1)=FN(H(J,1),FF(JN,1))
                  R=Q(J,1)-(D(J,1)*T(JN,1)+E(J,1)*T(J,1)+H(J,1)*T(J,2))
                  RR=ABS(R)
                  IF(RR.GT.RESID) RESID=RR
                  U(J, 1) = (R - CC * U(JN, 1)) / DD
                  IF(ABS(U(J,1)).LT.1.E-7) U(J,1)=0.
                 ALL ROWS EXCEPT ROW KNAX
                 DO 120 K=2,KMAXX
                 KP=K+1
                 KH=K-1
C
C
                  THE LEFT BURDER POINT
                 BB=BN(B(1,K),EE(1,KN))
                 DD=E(1,K)+DN1(EE(1,KN),FF(1,KN))
                 EE(1,K)=EN(F(1,K),EE(1,KN))
                 FF(1,K)=H(1,K)/DD
                 R=Q(1,K)+(B(1,K)*T(1,K))+E(1,K)*T(1,K)+F(1,K)*T(2,K)+H(1,K)*
               &T(1,KP))
                 RR=ABS(R)
                 IF(RR.GT.RESID) RESID=RR
                 U(1,K)=(R-BB*U(1,KN))/DD
                 IF(ABS(U(1,K)).LT.1.E-7) U(1.K)=0.
CCC
                 THE RON K EXCLUDING THE RIGHT BORDER POINT.
                 00 110 J=2, JMAXX
                 JP=J+1
                 JN=J-1
```

```
BB=BN(B(J,K),EE(J,KN))
      CC=CN(D(J,K),FF(JN,K))
      DD=E(J,K)+DH1(EE(J,KN),FF(J,KN))+DH2(FF(JN,K),EE(JN,K))
      EE(J,K)=EN(F(J,K),EE(J,KN))
      FF(J,K)=FN(H(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)+
     &F(J,K)*T(JP,K)+H(J,K)*T(J,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
  110 IF(ABS(U(J,K)),LT.1.E-7) U(J,K)=0.
C
CCC
      THE RIGHT BORDER POINT
      J=JMAX
      XXAML=HL
      BB=BN(B(J,K),EE(J,KN))
      CC=CN(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J.K)=0
      FF(J,K)=FN(H(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)*T(J,K)+H(J,K)*
     &T(J,KP))
      RR=ABS(R)
      IF (RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
  120 IF(ABS(U(J,K)).LT.1.E-7) U(J,K)=0.
000
      THE CORNER POINT (1.KNAX)
      K=KMAX
      KN=KMAXX
      BB=BN(B(1,K),EE(1,KN))
      DD=E(1,K)+DN1(EE(1,KN),FF(1,KN))
      EE(1,K)=EN(F(1,K),EE(1,KN))
      FF(1,K)=0
      R=R(1,K)-(B(1,K)*T(1,KN)+E(1,K)*T(1,K)+F(1,K)*T(2,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(1,K)=(R-BB*U(1,KN))/DD
      IF(ABS(U(1,K)).LT.1.E-7) U(1,K)=0.
CCC
      THE RON KMAX, EXCLUDING THE CORNER POINT (JMAX,KMAX)
      DO 130 J=2, JMAXX
      JP=J+1
      JN=J-1
      BB=BN(B(J,K),EE(J,KN))
      CC=CN(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J,K)=EN(F(J,K),EE(J,KN))
      FF(J,K)=0
      R=R(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)*T(J,K)+F(J,K)*
     &T(JP,K)
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
```

```
U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
  130 IF(ABS(U(J.K)) LT.1.E-7) U(J.K)=0.
CCC
      THE CORNER POINT (JMAX, KMAX)
      J=JMAX
      XXAML=NL
      BB=BN(B(J,K),EE(J,KN))
      CC=CN(D(J,K),FF(JN,K))
      DD=E(J,K)+DN1(EE(J,KN),FF(J,KN))+DN2(FF(JN,K),EE(JN,K))
      EE(J,K)=0
      FF(J,K)=0
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KN)-CC*U(JN,K))/DD
      IF(ABS(U(J,K)),LT,1,E-7) U(J,K)=0.
CCCCC
      INDEX K AND J IN REVERSE TO FIND DELTA
      THE CORNER POINT (JMAX, KMAX)
      K=KMAX
      DELTA(JMAX,K)=U(JMAX,K)
CCC
      THE ROW KMAX
      DO 140 JJ=1, JNAXX
      J=JMAXX+1-JJ
      JF = J+1
      DELTA(J,K)=V(J,K)-EE(J,K)*DELTA(JP,K)
  140 IF(ABS(DELTA(J,K)).LT.1.E-10) DELTA(J,K)=0.
CCC
      THE ROW K. TREATING THE RIGHT BORDER FIRST.
      DO 150 KK=1 KMAXX
      K=KMAXX+1-KK
      KP=K+1
      DELTA(JMAX,K)=U(JMAX,K)-FF(JMAX,K)*DELTA(JMAX,KP)
      IF(ABS(DELTA(JMAX,K)),LT.1.E-10) DELTA(JMAX,K)=0.
      00 150 JJ=1, JMAXX
      J=JMAXX+1-JJ
      JF = J+1
      DELTA(J,K)=U(J,K)-EE(J,K)*DELTA(JP,K)-FF(J,K)*DELTA(J,KP)
  150 IF(ABS(DELTA(J,K)).LT.1.E-10) DELTA(J,K)=0.
      GO TO 240
CCCCC
      ISTONE IS EVEN. INDEX K IN REVERSE ORDER.
      THE CORNER POINT (1,KMAX)
  170 K=KMAX
      KN=KMAXX
      DD=E(1.K)
      EE(1,K)=F(1,K)/DD
      FF(1,K)=B(1,K)/DD
```

```
R=Q(1,K)-(B(1,K)*T(1,KN)+E(1,K)*T(1,K)+F(1,K)*T(2,K))
      RR=ABS(R)
      RESID=RR
      U(1,K)=R/DD
      IF(ABS(U(1,K)).LT.1.E-7) U(1,K)=0
CC
      THE RON KMAX
      DO 180 J=2, JMAXX
      JP = J+1
      JH=J-1
      CC=CR(O(J,K),FF(JN,K))
      DD=E(J,K)+DR2(FF(JN,K),EE(JN,K))
      EE(J,K)=F(J,K)/DD
      FF(J,K)=FR(B(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)*F(J,K)+F(J,K)*
     &T(JP,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-CC*U(JN,K))/DD
  180 IF(ABS(U(J,K)).LT.1.E-7) U(J,K)=0
C
      THE CORNER POINT (JMAX, KNAX)
      J=JMAK
      XXAML=HL
      CC=CR(D(J,K),FF(JN,K))
      DD=E(J,K)+DR2(FF(JN,K),EE(JN,K))
      EE(J.K)=0
      FF(J,K) = FR(B(J,K), FF(JN,K))
      R=Q(J,K)+(B(J,K)*T(J,KN)*D(J,K)*T(JN,K)+E(J,K)*T(J,K))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-CC*U(JN,K))/DD
      IF(ABS(U(J,K)),LT,1,E-7) U(J,K)=0.
C
      ALL RONS EXCEPT THE ROW K=1
      00 200 KK=2 KMAXX
      K=KMAXX+2-KK
      KP=K+1
      KH=K-1
CC
      THE LEFT BURDER POINT (1.K)
      BB=BR(H(1,K),EE(1,KP))
      DD=E(1,K)+DR1(EE(1,KP),FF(1,KP))
      EE(1,K)=ER(F(1,K),EE(1,KP))
      FF(1,K)=B(1,K)/DD
      R=Q(1,K)+(B(1,K)*T(1,KN)+E(1,K)*T(1,K)+F(1,K)*T(2,K)+H(1,K)*
     &T(1,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID≃RR
      U(1,K)=(R-BB*U(1,KF))/DD
      IF(ABS(U(1,K)).LT.1.E-7) U(1,K)=0.
C
```

```
CC
      THE ROW K EXCLUDING THE RIGHT BORDER POINT
      DO 190 J=2, JMAXX
      JF= J+1
      JN= J-1.
      BB=BR(H(J,K),EE(J,KP))
      CC=CR(D(J,K),FF(JN,K))
      DD=E(J.K)+DR1(EE(J.KP),FF(J.KP))+DR2(FF(JN.K),EE(JN,K))
      EE(J,K)=ER(F(J,K),EE(J,KP))
      FF(J,K)=FR(B(J,K),FF(JN,K))
      R=R(J,K)-(B(J,K)*T(J,KN)+D(J,K)*T(JN,K)+E(J,K)*T(J,K)+F(J,K)*
     &T(JP,K)+H(J,K)*T(J,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KP)-CC*U(JN,K))/DD
  190 IF(ABS(V(J.K)).LT.1.E-7) V(J.K)=0
C
CC
      THE RIGHT BURDER POINT
      KAML=L
      JH=JMANN
      BB=BR(H(J,K),EE(J,KP))
      CC = CR(D(J,K),FF(JN,K))
      DD=E(J,K)+DR1(EE(J,KP),FF(J,KP))+DR2(FF(JN,K),EE(JN,K))
      EE(J,K)=0
      FF(J,K)=FR(B(J,K),FF(JN,K))
      R=Q(J,K)-(B(J,K)*T(J,KN)+Q(J,K)*T(JN,K)+E(J,K)*T(J,K)*T(J,K)+H(J,K)*
     &T(J,KP))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,K)=(R-BB*U(J,KP)-CC*U(JN,K))/BB
  200 IF(ABS(U(J,K)).LT.1.E-7) U(J,K)=0
\mathcal{C}
      THE CORNER POINT (1,1)
C
      BB=BR(H(1,1),EE(1,2))
      DD=E(1,1)+DR1(EE(1,2),FF(1,2))
      EE(1,1)=ER(F(1,1),EE(1,2))
      FF(1,1)=0
      R=R(1,1)-(E(1,1)*T(1,1)+F(1,1)*T(2,1)+H(1,1)*T(1,2))
      RR=ABS'R)
      IF(RR.GT.RESID) RESID=RR
      U(1,1)=(R-BB*U(1,2))/DD
IF(ABS(U(1,1)).LT.1.E-7) U(1,1)=0.
000
      THE ROW K=1, EXCLUDING THE RIGHT CORNER POINT.
      00 210 J=2, JMAXX
      JF = J + 1
      JN = J - 1
      BB=BR(H(J,1),EE(J,2))
      CC = CR(D(J, 1), FF(JN, 1))
      DD=E(J,1)+DR1(EE(J,2),FF(J,2))+DR2(FF(JN,1),EE(JN,1))
      EE(J,1)=ER(F(J,1),EE(J,2))
      FF(J, 1)=0
      R=R(J,1)-(D(J,1)*T(JH,1)+E(J,1)*T(J,1)+F(J,1)*T(JF,1)+H(J,1)*
     &T(J, 2))
```

```
RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,1)=(R-BB*U(J,2)-CC*U(JN,1))/DD
  210 IF(ABS(U(J,1)).LT.1.E-7) U(J,1)=0.
C
      THE CORNER POINT (JMAX, 1)
      J=JMAX
      JN=JMAXX
      BB=BR(H(J,1),EE(J,2))
      CC=CR(O(J,1),FF(JN,1))
      DD=E(J,1)+DR1(EE(J,2),FF(J,2))+DR2(FF(JN,1),EE(JN,1))
      EE(J,1)=0.
      FF(J,1)=0.
      R=R(J,1)-(D(J,1)*T(JN,1)+E(J,1)*T(J,1)+H(J/1)*T(J,2))
      RR=ABS(R)
      IF(RR.GT.RESID) RESID=RR
      U(J,1)=(R-BB*U(J,2)-CC*U(JN,1))/DD
      IF(ABS(U(J,1)).LT.1.E-7) U(J,1)=0.
CCCCC
      INDEX K FORWARD & J REVERSE TO FIND DELTA
      THE POINT (JMAX, 1)
      DELTA(JMAX,1)=U(JMAX,1)
CC
      THE ROW K=1
      DO 220 JJ=1, JNAXX
      J=JMAXX+1-JJ
      JP = J + 1
      DELTA(J,1)=V(J,1)-EE(J,1)*DELTA(JP,1)
  220 IF(ABS(DELTA(J,1)).LT.1.E-10) DELTA(J,1)=0.
CC
      ALL REMAINING ROWS
C
      DO 230 K=2,KMAX
      KH=K-1
CC
      THE RIGHT BORDER POINT
      DELTACINAX, K)=UCJMAX, K)-FFCJMAX, K)*DELTACJMAX, KN)
      IF(ABS(DELTA(JMAX,K)),LT.1.E-10) DELTA(JMAX,K)=0.
c
      ALL REMAINING POINTS OF THE ROW
      DO 238 JJ=1, JMAXX
      J=JMAXX+1-JJ
      JP=J+1
      DELTA(J,K)=U(J,K)-EE(J,K)*DELTA(JP,K)-FF(J,K)*DELTA(J,KN)
  230 IF(ABS(DELTA(J,K)).LT.1.E-10) DELTA(J,K)=0.
CCC
      CALCULATE NEW T(J,K)
  240 DO 250 J=1, JMAX
      DO 250 K=1 KMAX
```

```
250 T(J,K)=T(J,K)+DELTA(J,K)
      RETURN
CCC
      ENTRY STONE1 SETS UP ALPHA VALUES & INITIALIZES ALL ARRAYS
      ENTRY STONE1(JNAX, KMAX)
C
      DO 320 J=2, JMAX
      DO 320 K=2,KMAX
      DX=XDLT(J)/XPOS(JMAX)
      DY=YOLT(K)/YPOS(1)
  320 EE(J,K)≈2.E0/(1.E0/(DX*DX)+1.E0/(DY*DY))
CCC
      FIND AVERAGE
      ALPHX=0
      00 330 J=2,JMAX
      DO 330 K=2,KMAX
  330 ALPHX=ALPHX+EE(J,K)
      ALPHX=ALPHX/(JMAX*KMAX)
CCC
      IMPLEMENT STONE'S EQ(27)
      DO 348 J=1,9
      ALPHY=J-1
      ALPHY=ALPHY/8.E0
  340 EE(J,1)=ALPHX**ALPHY
0000
      IMPLEMENT THE SEQUENCE OF 18 ALPHAS SUGGESTED BY STONE
      ALPHA(1)=EE(9,1)
      ALPHA(3)=EE(6,1)
      ALPHA(5)=EE(3,1)
      ALPHA(7)=EE(8,1)
      ALPHA(9)=EE(5,1)
      ALPHA(11)=EE(2,1)
      ALPHA(13)=EE(7,1)
      ALPHA(15)=EE(4,1)
      ALPHA(17)=EE(1,1)
      DO 350 J=2,18,2
  350 ALPHA(J)=ALPHA(J-1)
      DO 360 J=1.18
  360 ALPHA(J)=1.E0-ALPHA(J)
00000
      INITIALIZE ALL ARRAYS INTERNAL TO STONE TO ZERO.
      00 370 J=1, JMAX
      DO 370 K=1,KMAX
      EE(J,K)=0.
      FF(J,K)=0.
      U(J,K)=0.
  370 DELTA(J,K)=0.
      RETURN
      END
C
```

```
SUBROUTINE EFIELD
CCCCC
      CALCULATES THE ELECTRIC FIELD COMPONENTS ESUBY & ESUBY
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
   % &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HHRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YOEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH
      COMMON/CHTRL/ITMAX/ITRNAX/CONURG/SIOLT
      ℃ONMON/NRNLZE/DNSNRM,PSINRM,DSTNRM,BLTZMN
CC
      ESUBX COMPONENT
      IMAXX=IMAX-1
      DO 140 I=2, IMAXX
      00 140 J=2, JMAX
      XW=XDLT(I)
      IF(IDENT(I,J).LT.0) GO TO 140
      IF(IDENT(I)J).EQ.0) GO TO 120
      IF(J.EQ.JNAX) GO TO 100
      YAU=(YDLT(J+1)+YDLT(J))/2.E0
      GO TO 110
  100 YAU=YDLT(J)
  110 XN=YAU/HWEST(I,J)
  120 ESUBX(I,J)=((PSI(I,J)-PSI(I+1,J))/XDLT(I+1)+(PSI(I-1,J)-PSI(I,J))
     &/XW)/2.E0
  140 CONTINUE
CC
      ESUBY COMPONENT
      JNAXX=JNAX-1
      DO 190 I=1, IMAXX
      DO 190 J=2, JMAXX
      YN=YDLT(J+1)
      IF(IDENT(I,J).LT.0) GO TO 190
      IF(IDENT(I,J),EQ.0) GO TO 170
      IF(I.EQ.1) GO TO 150
      XAU=(XDLT(I)+XDLT(I+1))/2.E0
    ~ GO TO 160
 150 XAU=XDLT(2)
  160 YN=XAU/HNRTH(I,J)
  170 ESUBY(I, J)=((PSI(I, J+1)-PSI(I, J))/YN+(PSI(I, J)-PSI(I, J-1))/
     &YOLT(J))/2.E0
  190 CONTINUE
      APPLY QUADRATIC EXTRAPOLATION TO FILL IN ESUBX & ESUBY AT THE
      EXTERNAL POINTS BORDERING THE INTERFACE.
      DO 200 I=1, IMAX
      DO 200 J=1, JMAX
```

```
IF(IDENT(I,J).GE.0) GO TO 200
    IF(IDENT(I+1, J).LT.0) GO TO 200
   DENOM=XDLT(I+3)*XDLT(I+2)*(XDLT(I+3)+XDLT(I+2))
   XX=XDLT(I+2)+XDLT(I+1)
   DENUM=XOLT(I+2)*ESUBX(I+3,J)+XOLT(I+3)*ESUBX(I+1,J)-
   &(XDLT(I+2)+XDLT(I+3))*ESUBX(I+2,J)
   AA=DENUM/DENOM
   DENUM=XDLT(I+2)*XDLT(I+2)*ESUBX(I+3,J)-XDLT(I+3)*XDLT(I+3)*
   &ESUBX(I+1,J)-(XDLT(I+2)*XDLT(I+2)-XDLT(I+3)*XDLT(I+3))*
  &ESUBX(I+2,J)
   BB=DENUM/DENOM
   ESUBX(I,J)=ESUBX(I+2,J)+AA*XX*XX-BB*XX
   DENON=YOLT(J-2)*YOLT(J-1)*(YOLT(J-2)+YOLT(J-1))
   XX=YDLT(J-1)+YDLT(J)
   DENUM=YDLT(J-1)*ESUBY(I,J-3)+YDLT(J-2)*ESUBY(I,J-1)-
   &(YDLT(J-1)+YDLT(J-2))*ESUBY(I,J-2)
   AA=DENUM/DENOM
   DENUM=YOLT(J-1)*YOLT(J-1)*ESUBY(I,J-3)-YOLT(J-2)*YOLT(J-2)*
   &ESUBY(I, J-1)-(YDLT(J-1)*YDLT(J-1)-YDLT(J-2)*YDLT(J-2))*
   &ESUBY(I, J-2)
    BB=DENUM/DENOM
    ESUBY(I.J)=ESUBY(I.J-2)+AA*XX*XX-BB*XX
200 CONTINUE
   RETURN
   END
```

CC

c	SUBROUTINE AVENCH(VETDET, AVDET, XPATH, YPATH, ET, KNTMAX)
000000	EVALUATES THE BREAKDOWN VOLTAGE AFTER LOCATING THE TRAJECTORY ALONG WHICH THE IONIZATION INTEGRAL IS A MAXIMUM.
c	COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31), &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31), &DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31), COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31), &HHRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31), COMMON/REAL/XWIDTH,YDEPTH,BRRIER,EGAP,TMPTR,ACCPTR,VBLTIN,VOLT, &TRNSIC,QSS,XØ,YØ,RAD,XDELTA,YDELTA COMMON/INTGR/IMAX,JMAX,IXWDTH,JYDPTH COMMON/CNTRL/ITMAX,ITRMAX,CONURG,SIDLT COMMON/NRMLZE/DHSNRM,PSINRM,DSTNRM,BLTZMN COMMON/RSCALE/ RSFCTR
	DIMENSION XSTART(3), YSTART(3), PI(3), KNTMX(3), ISTART(3), JSTART(3) DIMENSION XPATH(KNTMAX,3), YPATH(KNTMAX,3), ET(KNTMAX,3)
00000	CALCULATE EQUILIBRIUM PARAMETERS. ESTIMATE THE BREAKDOWN VOLTAGE, AND CALCULATE INITIAL NORMALIZATIONS.
·	CALL EQULIB  CALL UGUESS(VOLT)  WRITE(6,900) VOLT  900 FORMAT(2X,//,2X,'THE INITIAL VOLTAGE ESTIMATE IS',1PE10.2,  &1X,'VOLTS',//)  RSFCTR=1.0  RDSAVE=RAD  XWSAVE=XWIDTH  YDSAVE=YDEPTH  QSSAVE=QSS  PSINRM=VBLTIN+VOLT  DSTNRM=SQRT(2.*11.7*8.854E-14*PSINRM/(1.602E-19*DNSNRM))  KSWCH=0
	K=1 ISTART(2)=IXWOTH JSTART(2)=JYDPTH
CC	PROVIDE CURRENT HORMALIZATIONS OF RAD, XWIDTH, YDEPTH, & QSS
c	100 RAD=RDSAVE/(DSTHRM*1.E4) XWIDTH=XWSAVE/(DSTHRM*1.E4) YDEPTH=YDSAVE/(DSTHRM*1.E4) QSS=QSSAVE*DSTHRM/(11.7*8.854E-14*PSINRM) SIHRMO=PSIHRM
000000	USING PRESENT NORMALIZATIONS, SOLVE POISSON'S EQ. & OBTAIN THE ELECTRIC FIELD LATTICES. IF KSWCH.EQ.O, LOCATE POSITION OF MAX E-FIELD AND ESTABLISH THREE STARTING LOCATIONS CENTERED ABOUT THA POSITION. IF KSWCH.GT.O, ESTABLISH ONLY THE CENTRAL STARTING LOCATION.

```
C
      CALL GRID
      CALL STONE1(IMAX, JMAX)
      CALL BURDER
      CALL NITIAL
      CALL GRELAX
      CALL EFIELD
      I=ISTART(2)-1
      J=JSTART(2)-1
      IF(RAD.NE.XWIDTH.OR.RAD.NE.YDEPTH.OR.QSS.NE.0.) GO TO 105
      K=2
      KSWCH=1
      GO TO 120
  105 IF(KSWCH.GT.0) GO TO 120
      ETST=2.E5*DSTNRM/PSINRM
      ENAX=0.
      DO 110 II=1,IMAX
      DO 110 JJ=1. JMAX
      ETT=SQRT(ESUBX(II,JJ)*ESUBX(II,JJ)+ESUBY(II,JJ)*ESUBY(II,JJ))
      IF(ETT.LE.EMAX) GO TO 110
      EMAX=ETT
      I = II
      J=JJ
  118 CONTINUE
      IF(EMAX.GE.ETST) GO TO 115
      PSINRM=PSINRM*1.05*(ETST/EMAX)*(ETST/EMAX)
      DSTHRM=SQRT(2,*11,7*8.854E-14*PSIHRM/(1,602E-19*DHSHRM))
  115 I=I-2
      J=J-2
CC
      ESTABLISH STARTING COORDINATES FOR TRAJECTORY K.
  120 I=I+1
      J=J+1
      X=XPOS(I)
      Y=YPOS(J)
      IF(X.GT.X0) GO TO 125
      XSTART(K)=X
      YSTART(K)=YPOS(JYDPTH)
      GO TO 150
  125 IF(Y.GT.Y0) GO TO 130
      XSTART(K)=XPOS(IXWDTH)
      YSTART(K)=Y
      GO TO 150
  130 X=X-X0
      Y=Y-Y0
      IF(X.LT.Y) GO TO 140
      Y=Y/X
      XSTART(K)=X0+RAD/SQRT(1.E0+Y*Y)
      YSTART(K)=Y0+(XSTART(K)-X0)*Y
      GO TO 150
  148 X=X/Y
      YSTART(K)=Y0+RAD/SQRT(1.E0+X*X)
      XSTART(K)=X0+(YSTART(K)-Y0)*X
  150 IF(KSNCH.GT.0) GO TO 180
      K=K+1
```

```
IF(K.GT.3) GO TO 170
       GO TO 120
CC
       TRACE OUT THE TRAJECTORY FOR STARTING POSITION K.
  170 K=1
  180 KHT=1
      KEXIT=0
       X=XSTART(K)
       Y=YSTART(K)
       I = IXMDTH
       J=JYDPTH
       OLTX=X-XPOS(IXWOTH)
       DLTY=Y-YPOS(JYDPTH)
       CALL INDEX(I, J, DLTX, DLTY, KEXIT)
       ISTART(K)=I
       JSTART(K)=J
       IF(DLTX.LT.XDLT(I+1)/1.E3) DLTX=XDLT(I+1)/1.E3
IF(DLTY.LT.YDLT(J)/1.E3) DLTY=YDLT(J)/1.E3
       X=XPOS(I)+DLTX
       Y=YPOS(J)+DLTY
       CALL EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET(1, K))
      XPATH(1.K)=X
       YPATH(1,K)=Y
       ETT≈ET(1.K)
  190 CALL TRAJEC(KNT, I, J, X, Y, DLTX, DLTY, ETT, KEXIT)
       IF(KEXIT.GT.0) GO TO 200
       KNT=KNT+1
       IF(KNT.GT.KNTMAX) GO TO 195
      XPATH(KNT,K)=X
       YPATH(KNT,K)=Y
      ETCKNT,K)=ETT
       GO TO 190
  195 NRITE(6,1000) KNTMAX
 1000 FORMAT(1H1.30X,/,5X,'EXCEEDED STORAGE ALLOTTED FOR TRAJECTORIES
     &'(KNTMAX=',13,').';/,5X,'INCREASE THE VALUE OF THAT PARAMETER ',
     &'IN NAMELIST CONTRL. '. / 5X, 'INCREASE DIMENSIONS '
     & ALLOTED TO XPATH, YPATH, & ET IN MAIN, IF NECESSARY. ')
      STOP
  200 KNTMX(K)=KNT
      KNT=1
      PI(K)=0.
      XST=XSTART(K)*DSTNRM*1.E4
       YST=YSTART(K)*DSTNRM*1.E4
      XPT=XPATH(1,K)*DSTNRM*1.E4
       YPT=YPATH(1,K)*DSTNRM*1.E4
       EPT=ET(1,K)*PSINRM/DSTNRM
      WRITE(6, 1010)K, ISTART(K), JSTART(K), XST, YST, XPT, YPT, EPT, PI(K)
 1010 FORMAT(2X, //, 2X, 'K', 3X, 'ISTART', 1X, 'JSTART', 3X, 'XSTART', 4X,
     &'YSTART', 4X, 'XPATH', 5X, 'YPATH', 6X, 'ET', 7X, 'ALPHA', 5X, 'PI', //
     &1X, I2, 5X, I2, 5X, I2, 3X, 1P5E10.2, 10X, 1PE10.2)
CC
      EVALUATE THE IONIZATION INTOXZPF ALONG TRAJECTORY K.
  210 KHT=KHT+1
      IF(KNT.GT.KNTMX(K)) GO TO 220
```

```
DX=XPATH(KNT,K)-XPATH(KNT-1,K)
      DY=YPATH(KNT,K)-YPATH(KNT-1,K)
      ET2=ET(KNT,K)
      ET1=ET(KNT-1,K)
      PIO=PI(K)
      CALL INTGRL(DX,DY,ET1,ET2,PI(K),ALPHA)
      XPT=XPATH(KNT,K)*DSTNRM*1.E4
      YPT=YPATH(KNT,K)*DSTNRM*1.E4
      EPT=ET(KNT,K)*PSINRM/DSTNRM
      WRITE(6,1020)XPT,YPT,EPT,ALPHA,PI(K)
 1020 FORMAT(40X,1P5E10.2)
      TST=(PI(K)-PI0)/PI(K)
      IF(TST.GT.1.E-4) GO TO 210
  220 IF(KSNCH.GT.0) GO TO 230
      K=K+1
      IF(K.LT.4) GO TO 180
      KSWCH=1
  230 IF(K.EQ.2) GO TO 290
CCCC
      ADJUST STARTING POSITIONS UNTIL THE TRAJECTORY K=2 PRODUCES THE
      MAXIMUM IONIZATION INTEGRAL.
      IF(PI(1).GT.PI(2)) GO TO 250
      IF(K.EQ.1) GO TO 240
      IF(PI(3).GT.PI(2)) GO TO 270
  240 K=2
      GO TO 290
C
CCC
      MAXIMUM IS TO LEFT OF K=2. SHIFT LEFT ACCORDINGLY.
  250 K=1
      ISTART(2)=ISTART(1)
      JSTART(2)=JSTART(1)
      XSTART(2)=XSTART(1)
      YSTART(2)=YSTART(1)
      PI(2)=PI(1)
      KHTMX(2)=KHTMX(1)
      KMX=KNTMX(1)
      DO 260 KHT=1,KMX
      XPATH(KNT,2)=XPATH(KNT,1)
      YPATH(KNT,2)=YPATH(KNT,1)
  260 ET(KNT,2)=ET(KNT,1)
      I=ISTART(1)-2
      J=JSTART(1)-2
      IF(I.LT.0) GO TO 240
      GO TO 120
CC
      MAXIMUM IS TO RIGHT OF K=2. SHIFT RIGHT ACCORDINGLY.
  270 K=3
      ISTART(2)=ISTART(3)
      JSTART(2)=JSTART(3)
      XSTART(2)=XSTART(3)
      YSTART(2)=YSTART(3)
      PI(2)=PI(3)
      KHTMX(2)=KHTMX(3)
```

```
KMX=KNTMX(3)
      00 280 KHT=1.KMX
      XPATH(KNT,2)=XPATH(KNT,3)
      YPATH(KNT, 2)=YPATH(KNT, 3)
  280 ET(KHT,2)=ET(KHT,3)
      I=ISTART(3)
      J=JSTART(3)
      IF(J.EQ.JMAX) GO TO 240
      GO TO 120
000000
      ADJUST PSINRN UNTIL ONE MINUS PI CHANGES SIGN. THEN USE THE
      METHOD OF SECANTS TO FIND THE VALUE OF PSINRM LEADING TO
      BREAKDOWN.
  290 Y1=1.0-PI(2)
      X1=PSINRM
      KEY=1
      IF(Y1.GT.0.) GO TO 300
      FCTR=0.9E0
      GO TO 310
  300 FCTR=1.1E0
  310 X2=X1*FCTR
      GO TO 360
  320 Y2=1.0-PPI
      TST=Y1*Y2
      IF(TST.LT.0.) GO TO 330
      Y1=Y2
      X1=X2
      GO TO 310
000
      METHOD OF SECANTS.
  330 KEY=2
      KSEC=0
  340 DEN=Y2-Y1
      IF(ABS(Y2).LT.AUDLT) GO TO 380
      KSEC=KSEC+1
      XX=(X1*Y2-X2*Y1)/DEN
      X1=X2
      Y1=Y2
      X2=XX
      GO TO 360
  350 Y2=1.0-PPI
      GO TO 340
CCC
      SUBPROGRAM FOR THE IONIZATION INTEGRAL
  360 KNT=1
      PPI=0.
      PSINRM=X2
      DSTHRM=DSTHRM*SQRT(X2/X1)
      WRITE(6,1030) KEY, PSINRM, DSTNRM
 1030 FORMAT(1H0,2X,'KEY=',I2,6X,'PSINRM=',IPE11.3,3X,'OSTNRM=',
     &1PE11.3,//)
      WRITE(6, 1040)
 1040 FORMAT(1H0,2X, 'KNT',4X, 'DX',8X, 'DY',8X, 'ET1',7X, 'ET2',
     &7X, 'ALPHA', 5X, 'PI', //)
```

```
370 KNT=KNT+1
      FFI0=FFI
      IF(KNT.GT.KNTMX(2)) GO TO (320,350), KEY
      DX=XPATH(KNT,2)-XPATH(KNT-1,2)
      DY=YPATH(KNT,2)-YPATH(KNT-1,2)
      ET2=ET(KNT,2)
      ET1=ET(KNT-1,2)
      CALL INTGRL(DX,DY,ET1,ET2,PPI,ALPHA)
      DXX=DX*DSTNRM
      DYY=DY*DSTNRM
      ETT1=ET1*PSINRM/DSTNRM
      ETT2=ET2*PSINRM/DSTNRM
      WRITE(6,1050) KNT, DXX, DYY, ETT1, ETT2, ALPHA, PPI
 1050 FORMAT(2X, I3, 1X, 1P6E10.2)
      TST=(PPI-PPI0)/PPI
      IF(TST.LT.1.E-4) GO TO(320,350),KEY
      GO TO 370
000000
      TEST FOR CONVERGENCE OF PSINRM. IF NOT, FIND NEW SOLUTION OF
      POISSON'S EQ & REEVALUATE THE VALUE OF PSINRM REQUIRED FOR BREAK-
      DOWN. IF SO, RENORMALIZE RAD, XWIDTH, YDEPTH, & QSS FOR THE
      PURPOSE OF PROVIDING CORRECT OUTPUT DATA ON DIMENSIONS.
  380 TST=ABS((PSINRM-SINRM0)/SINRM0)
      WRITE(6,1060) KSEC
 1060 FORMAT(2X,//,2X,I3,1X,'ITERATIONS WERE REQUIRED WITH THE METHOD',
     &1X, 'OF SECANTS IN AULNCH',//)
      IF(TST.LE.VLTDLT) GO TO 390
      GO TO 100
  390 RAD=RDSAVE/(DSTNRM*1.E4)
      XWIDTH=XWSAVEZ(DSTNRM*1.E4)
      YDEPTH=YDSAVE/(DSTNRM*1.E4)
      QSS=QSSAVE*DSTNRM/(11.7*8.854E-14*FSINRM)
      CALL GRID
      CALL STONE1(IMAX, JMAX)
      CALL BORDER
      CALL NITIAL
      CALL GRELAX
      CALL EFIELD
      RETURN
      END
C
```

000000

SUPPLIES INITIAL ESTIMATE OF THE BREAKDOWN VOLTAGE USING AN EMPIRICAL FIT TO THE KENNEDY-O'BRIEN CURVES.

COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31), &D(31,31), E(31,31), F(31,31), F(31,31), Q(31,31), Q(31,31), QAREA(31,31), &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31), HEAST(31,31), COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31), &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31), COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, UOLT, &TRNSIC, QSS, XO, YO, RAD, XDELTA, YDELTA COMMON/INTGR/IMAX, JMAX, IXWDTH, JYDPTH COMMON/CNTRL/ITMAX, ITRMAX, CONURG, SIDLT COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN

c

RR=RAD IF(RR.EQ.0) RR=0.1 AA=1./(18.+150.\*RR) UNIT=1./(AA+3.75E-12\*DNSNRM\*\*0.6) AA=2.303E4/(DNSNRM\*\*.3695) BB=7.891E3/(DNSNRM\*\*.2968) TT=TMPTR/300.-1. UNIT=UNIT\*(AA\*TT\*TT+BB\*TT+1.) RETURN END

C

## SUBROUTINE EQULIB

```
CCCCCCCC
       USING UNNORMALIZED VARIABLES, CALCULATES THE TEMPERATURE-
      DEPENDENT BAND GAP, THE IONIZED ACCEPTOR DENSITY, AND THE BUILT-IN POTENTIAL BARRIER, ACCOUNTING FOR THE TEMPERATURE DEPENDENCE OF
       THE INTRINSIC DENSITY AND OF THE FERMI LEVEL.
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
       COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT,
     &TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
      COMMONZINTGRZIMAX, JMAX, IXNOTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONVRG, SIDLT
      COMMON/NRMLZE/DNSNRM, PSINRM, DSTNRM, BLTZMN
      COMMON/SWICH/ NOOPE
C
       T=TMPTR/3.E2
      BLTZMN=0.02585*T
      EGAP=1.165-7.242E-3*T-3.664E-2*T*T
      EIU=EGAP/2.E0-1.306E-2*T
      X = EIU
      KEY=1
      GO TO 178
000
      ADJUST X18X2 UNTIL Y18Y2 HAVE OPPOSITE SIGN
  100 X1=X
      Y1=Y
      DX = -EIU/2.E1
      IF(Y,LT,\theta,) DX=-DX
      X=X1+DX
      KEY=2
      GO TO 170
  110 X2=X
      Y2=Y
      IF(Y1*Y2.LE.0.) GO TO 140
  130 X1=X2
      Y1=Y2
      X=X2+DX
      GO TO 170
  140 KEY=3
CCC
      METHOD OF SECANTS
  150 IF(ABS(Y).LT.1.E-3) GO TO 180
      DEN=Y2-Y1
      X=(X1*Y2-X2*Y1)/DEN
      GO TO 170
  160 X1=X2
      Y1=Y2
      X2=X
```

```
Y2=Y
       GO TO 150
000
       SUBROUTINE FOR EVALUATING Y
  170 EIF=X
       EFU=EIU-EIF
       EAF=4.38E-2-3.037E-8*ACCPTR**(1.0/3.0)-EFU
       BKGRND=ACCPTR/(1.0+(4.0+2.0/EXP(4.4E-2/BLTZMN))*EXP(EAF/BLTZMN))
       IF(NOOPE.GT.0) BKGRND=ACCPTR/(1.+2.*EXP(EAF/BLTZMN))
       TRNSIC=3.925E19*T*SQRT(T)*EXP(-EGAP/(2.*BLTZMN))
       BULKP=TRNSIC*EXP(EIF/BLTZMN)
       Y=(BULKP-BKGRND)/ACCPTR
       GO TO(100,110,160), KEY
CCCC
       CALCULATE THE BUILTIN POTENTIAL, THE ELECTRON DENSITY AT THE
       METAL-SILICON INTERFACE, AND THE BULK HOLE DENSITY.
  180 UBLTIN=BRRIER-EFU
       DNSNRM=BKGRND
       WRITE(6,1000)TMPTR, EGAP, EIU, EIF, EFU, TRNSIC, BKGRND, UBLTIN
 1000 FORMAT(2X,//,3X,'TMPTR',5X,'EGAP',7X,'EIV',7X,'EIF',7X,'EFU',
&6X,'TRNSIC',4X,'BKGRND',4X,'UBLTIN',//,1X,1P8E10.2,//)
       RETURN
       END
CC
```

C

TRACKS WHICH 'BOX' OF THE LATTICE IS OCCUPIED BY THE MOVING CHARGE & SUPPLIES ITS INDICES (I,J) AND CORRECT VALUES FOR DLTX & DLTY WITH RESPECT TO THAT POINT. ALSO FLAGS AN EXIT OF THE CHARGE FROM THE REGION.

COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),B(31,31),
&D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
&DELTA(31,31),ESUBX(31,31),ESUBY(31,31),IDENT(31,31),
COMMON/COEFF/HSTH(31,31),HWEST(31,31),HCNTR(31,31),HEAST(31,31),
&HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
COMMON/REAL/XWIDTH,YDEPTH,BRRIER,EGAP,TMPTR,ACCPTR,VBLTIN,VOLT,
&TRNSIC,QSS,X0,Y0,RAD,XDELTA,YDELTA
COMMON/INTGR/IMAX,JMAX,IXWDTH,JYDPTH
COMMON/CNTRL/ITMAX,ITRMAX,CONVRG,SIDLT
COMMON/HRMLZE/DNSHRM,PSINRM,DSTNRM,BLTZMN

IF(DLTX.LT.0.) GO TO 100 IF(DLTX.GT.XDLT(I+1)) GO TO 110 GO TO 120

100 IF(I.EQ.1) GO TO 150

OLTX=XDLT(I)+DLTX

I=I-1

IF(DLTX.LT.0.) GO TO 100

GO TO 120

110 IF(I.EQ.(IMAX-1)) GO TO 150 DLTX=DLTX-XDLT(I+1) I=I+1 IF(DLTX.GT.XDLT(I+1)) GO TO 110

120 IF(DLTY.LT.0.) GO TO 130 IF(DLTY.GT.YDLT(J)) GO TO 140 RETURN

130 IF(J.EQ.JMAX) GO TO 150
DLTY=YDLT(J+1)+DLTY
J=J+1
IF(DLTY.LT.0.) GO TO 130

RETURN

140 IF(J.EQ.2) GO TO 150

DLTY=DLTY-YDLT(J)

J=J-1

IF(DLTY.GT.YDLT(J)) GO TO 140

RETURN

150 KEXIT=1 RETURN END

C

ET=SQRT(EX\*EX+EY\*EY)

RETURN END

C

```
SUBROUTINE TRAJEC(KNT, I, J, X, Y, DLTX, DLTY, ET, KEXIT)
      USES ADAMS-BASHFORTH-MOULTON PREDICTOR-CORRECTOR EQ'S TO TRACE
0000000
      HOLE TRAJECTORIES, FOLLOWING A FOURTH-ORDER RUNGE-KUTTA STARTING
      PROCEDURE.
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31), XDLT(32), YDLT(32), XPOS(31), YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, VBLTIN, VOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JNAX, IXNDTH, JYDPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONVRG, SIDLT
      COMMON/HRMLZE/DNSHRM, PSINRM, DSTNRM, BLTZMN
C
      DIMENSION DX(7), DY(7)
C
      IF(KNT.GT.4) GO TO 100
      IF(KNT.GT.1) GO TO 90
      DLTA=0.005
      TOELT=DLTA/ET
      DO 80 K=1,7
      DX(K)=\emptyset.
   80 DY(K)=0.
000
      RUNGE-KUTTA PROCEDURE
   90 CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      CALL EFORCE(I, J, X, Y, DLTX, DLTY, EX, EY, ET)
      DX1=EX*TDELT
      DY1=EY*TDELT
      XX=X+DX1/2.E0
      YY=Y+0Y1/2.E0
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      CALL EFORCE(I, J. XX, YY, DLTX, DLTY, EX, EY, ET)
      DX2=EX*TDELT
      DY2=EY*TDELT
      XX=X+DX2/2.E0
       YY=Y+DY2/2.E0
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX3=EX*TDELT
      DY3=EY*TDELT
      XX=X+DX3
      YY=Y+DY3
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
```

```
CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
    DX4=EX*TDELT
    DY4=EY*TOELT
    DX(KNT+3)=(DX1+2.E0*(DX2+DX3)+DX4)/6.E0
    DY(KNT+3)=(DY1+2.E0*(DY2+DY3)+DY4)/6.E0
    X=X+DX(KNT+3)
    Y=Y+DY(KNT+3)
    DLTX=X-XPOS(I)
    DLTY=Y-YPOS(J)
    CALL INDEX(I, J, DLTX, DLTY, KEXIT)
    CALL EFORCE(I, J, X, Y, OLTX, DLTY, EX, EY, ET)
    DXCKNT+3)=EX*TDELT
    DY(KNT+3)=EY*TDELT
    KOBLE=3
    RETURN
    PREDICTOR-CORRECTOR, USING THE PRESENT INTERVAL
100 XPROCT=(55.E0*DX(7)-59.E0*DX(6)+37.E0*DX(5)-9.E0*DX(4))/24.E0
    YPRDCT=(55.E0*DY(7)-59.E0*DY(6)+37.E0*DY(5)-9.E0*DY(4))/24.E0
    XX=X+XPROCT
    YY=Y+YPROCT
    DLTX=XX-XPOS(I)
    DLTY=YY-YPOS(J)
    CALL INDEX(I, J, DLTX, DLTY, KEXIT)
    IFCKEXIT.GT.0) RETURN
    CALL EFORCE(I,J,XX,YY,DLTX,DLTY,EX,EY,ET)
    DX1=EX*TDELT
    DY1=EY*TDELT
    XCRRCT=(9.E0*0X1+19.E0*0X(7)-5.E0*0X(6)+0X(5))/24.E0
    YCRRCT=(9.E0*DY1+19.E0*DY(7)-5.E0*DY(6)+DY(5))/24.E0
    DX2=ABS(XPRDCT-XCRRCT)
    DY2=ABS(YPRDCT-YCRRCT)
    DLT=AMAX1(DX2,DY2)
    HALUE THE INTERVAL IF DLT EXCEEDS DLTA
    IF(DLT.LT.DLTA) GO TO 110
   PARABOLIC INTERPOLATION COEFFICIENTS FOR THE HALF INTERVAL VALUES
   KOBLE=3
    TOELT=TOELT/2.E0
   AA=(DX(7)-2.E0*DX(6)+DX(5))/(8.E0*TDELT*TDELT)
   BB=(DX(7)-DX(5))/(4.E0*TDELT)
    AAA=(DX(6)-2.E0*DX(5)+DX(4))/(8.E0*TDELT*TDELT)
   BBB=(DX(6)-DX(4))/(4.E0*TDELT)
   DX(1)=DX(4)/2.E0
   DX(3)=DX(5)/2.E0
   DX(5)=DX(6)/2.E0
   DX(2)=(TOELT*(AAA*TDELT-BBB)+DX(3))/2.E0
   DX(4)=(TOELT*(AA*TOELT-BB)+DX(5))/2.E0
   DX(6)=(TDELT*(AA*TDELT+BB)+DX(5))/2.E0
   DX(7)=DX(7)/2.E0
   AA=(DY(7)-2.E0*DY(6)+DY(5))/(8.E0*TDELT*TDELT)
BB=(DY(7)-DY(5))/(4.E0*TDELT)
```

```
AAA=(DY(6)-2.E0*DY(5)+DY(4))/(8.E0*TDELT*TDELT)
      BBB=(DY(6)-DY(4))/(4.E0*TDELT)
      DY(1)=DY(4)/2.E0.
      DY(3)=DY(5)/2.E0
      DY(5)=DY(6)/2.E0
      DY(2)=(TDELT*(AAA*TDELT-BBB)+DY(3))/2.E0
      DY(4)=(TDELT*(AA*TDELT-BB)+DY(5))/2.E0
      DY(6)=(TDELT*(AA*TDELT+BB)+DY(5))/2.E0
      DY(7)=DY(7)/2.E0
      GO TO 100
00000
      TENTATIVELY DOUBLE THE INTERVAL, BUT ONLY IF 3 STEPS HAVE BEEN
      TAKEN SINCE THE LAST DOUBLING OR HALVING, AND ONLY IF DLT
      IS LESS THAN ONE HALF OF DLTA
  110 IF(KOBLE.GT.0) GO TO 120
      DLT=DLT#2.0
      IF(DLT.GT.DLTA) GO TO 120
      XPRDT=(55.E0*DX(7)-59.E0*DX(5)+37.E0*DX(3)-9.E0*DX(1))/12.E0
      YPRDT=(55, E0*DY(7)-59, E0*DY(5)+37, E0*DY(3)-9, E0*DY(1))/12, E0
      XX=X+XPROT
      YY=Y+YPRDT
      DLTX=XX-XPOS(I)
      DLTY=YY-YPOS(J)
      CALL INDEX(I, J, DLTX, DLTY, KEXIT)
      IF(KEXIT.GT.0) GO TO 120
      CALL EFORCE(I, J, XX, YY, DLTX, DLTY, EX, EY, ET)
      DX1=EX*TDELT
      DY1=EY*TDELT
      XCRRT=(9.E0*DX1+19.E0*DX(7)-5.E0*DX(5)+DX(3))/12.E0
      YCRRT=(9.E0*DY1+19.E0*DY(7)-5.E0*DY(5)+DY(3))/12.E0
      DX2≈ABS(XPRDT-XCRRT)
      DY2=ABS(YPRDT-YCRRT)
      DLT=AMAX1(DX2,DY2)
      IF(DLT.GT.DLTA) GO TO 120
CCC
      DOUBLE INTERVAL IS OK, SO DO IT
      DX(7)=DX(7)*2.E0
      DX(6)=DX(5)*2.E0
      DX(5)=DX(3)*2.E0
      DX(4)=DX(1)*2.E0
      DY(7)=DY(7)*2.E0
      DY(6)=DY(5)*2.E0
      DY(5)=DY(3)*2.E0
      DY(4)=DY(1)*2.E0
      X=X+(19.E0*XPROT+251.E0*XCRRT)/270.E0
      Y=Y+(19.E0*YPRDT+251.E0*YCRRT)/270.E0
      TDELT=2.E0*TDELT
      KOBLE=3
      GO TO 130
CCC
      NO DOUBLING OCCURRED. COMPUTE NEW X % Y. SHIFT INCREMENTS LEFT
      & UPDATE THE MOST RECENT INCREMENT.
  120 X=X+(19.E0*XPRDCT+251.E0*XCRRCT)/270.E0
```

```
Y=Y+(19.E0*YPRDCT+251.E0*YCRRCT)/270.E0
KDBLE=KDBLE-1

130 DO 140 K=1.6
DX(K)=DX(K+1)

140 DY(K)=DY(K+1)
DLTX=X-XPOS(I)
DLTY=Y-YPOS(J)
CALL INDEX(I,J,DLTX,DLTY,KEXIT)
IF(KEXIT.GT.0) RETURN
CALL EFORCE(I,J,X,Y,DLTX,DLTY,EX,EY,ET)
ETT=ET*PSINRM/DSTNRM
IF(ETT.LT.2.E4) KEXIT=1
DX(7)=EX*TDELT
DY(7)=EY*TDELT
RETURN
END
```

```
SUBROUTINE INTGRL(DX,DY,E1,E5,PI,ALPHA)
CCC
      USES THE KENNEDY IONIZATION COEFFICIENT (AT 300 DEG K), SCALED TO
      THE TEMPERATURE T USING CROWELL & SZE'S EMPIRICAL FIT TO BARAFF'S CURVES, TO EVALUATE THE IONIZATION INTEGRAL BY GAUSSIAN QUADRATURE
C
      COMMON/ARRAYS/PSI(31,31), EDENS(31,31), HDENS(31,31), B(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31).
      COMMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31),XDLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      COMMON/INTGR/IMAX, JMAX, IXNOTH, JYOPTH
      COMMON/CHTRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/HRMLZE/DHSHRM, PSINRM, DSTNRM, BLTZMN
C
      DS=SQRT(DX*DX+DY*DY)*DSTNRM
      DZ=DS*A1/2.
      AA=(E5-E1)/DS
      BB=(E5+E1)/2.
      E2=(-AA*DZ+BB)*PSINRM/DSTNRM
      E3≈BB*PSINRM/DSTNRM
      E4≈(AA*DZ+BB)*PSINRM/DSTNRM
      AA=1.47E6
      BB=1.875E6
      ET=E2
      ALPHA=AA/EXP(BB/E2)
      KEY=1
      GO TO 130
  100 PI=PI+ALPHA*H1*DS/2.
      ET=E3
      ALPHA=AA/EXP(BB/E3)
      KEY=2
      GO TO 130
  110 PI=PI+ALPHA*H2*DS/2.
      ET=E4
      ALPHA=AA/EXP(BB/E4)
      KEY=3
      GO TO 130
  120 PI=PI+ALPHA*H1*DS/2.
      RETURN
  130 IF(TMPTR.EQ.300.) GO TO(100,110,120),KEY
      BLTZ= . 02585
      CALL CRUSZE(ET, BLTZ, ALPH)
      RATIO=ALPHA/ALPH
      BLTZ=BLTZMN
      CALL CRWSZE(ET,BLTZ,ALPH)
      ALPHA=RATIO*ALPH
      GO TO(100,110,120),KEY
      ENTRY INTGRI
      A1=.774596669241483
      H1 = .55555555555556
```

H2=.88888888888889

RETURN END SUBROUTINE CRWSZE(ET, BLTZ, ALPH)

```
CCC
      COMMON/ARRAYS/PSI(31,31),EDENS(31,31),HDENS(31,31),8(31,31),
     &D(31,31),E(31,31),F(31,31),H(31,31),Q(31,31),QAREA(31,31),
     &DELTA(31,31), ESUBX(31,31), ESUBY(31,31), IDENT(31,31)
      CONMON/COEFF/HSTH(31,31), HWEST(31,31), HCNTR(31,31), HEAST(31,31),
     &HNRTH(31,31),XOLT(32),YDLT(32),XPOS(31),YPOS(31)
      COMMON/REAL/XWIDTH, YDEPTH, BRRIER, EGAP, TMPTR, ACCPTR, UBLTIN, VOLT,
     &TRNSIC, QSS, X0, Y0, RAD, XDELTA, YDELTA
      CONMON/INTGR/IMAX, JMAX, IXNOTH, JYOPTH
      COMMON/CHIRL/ITMAX, ITRMAX, CONURG, SIDLT
      COMMON/NRMLZE/DHSHRM, PSINRM, DSTNRM, BLTZNN
      DIMENSION SCRICH(31), X(31), Y(31)
      DO 80 I=1, IMAX
   80 X(I)=XPOS(I)*DSTNRM*1.0E4
      DO 90 J=1.JMAX
   90 Y(J)=YPOS(J)*DSTNRM*1.0E4
      WRITE(6,1000)
 1000 FORMAT(1H1,60X,/,32X,'X(I),I=1,IMAX',//)
      WRITE(6,1010)(X(I),I=1,IMAX)
 1010 FORMAT(32X, 1P10E10.2)
      WRITE(6, 1020)
 1020 FORMAT(1H0,5X,'J',9X,'Y(J)',15X,'PSI(I,J),I=1,IMAX',//)
      DO 110 JJ=1. JMAX
      J=JMAX+1-JJ
      DO 100 I=1. IMAX
  100 SCRTCH(I)=PSI(I,J)*PSINRN
      WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
      WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
 1030 FORMAT(1X, ' ', /, 17, 5X, 1PE10.2, 10X, 1P10E10.2)
 110 CONTINUE
 1040 FORMAT(32X, 1F10E10.2)
      WRITE(6, 1000)
      WRITE(6,1010)(X(I),I=1,IMAX)
      WRITE(6, 1060)
 1060 FORMAT(1H0,5X,'J',9X,'Y(J)',15X,'HDENS(I,J),I=1,IMAX',//)
      DO 150 JJ=1, JMAX
      J=JMAX+1-JJ
      DO 140 I=1, IMAX
  140 SCRTCH(I)=HDENS(I,J)*DNSNRM
      WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
      WRITE(6,1040)(SCRTCH(I),I=11,INAX)
  150 CONTINUE
      WRITE(6, 1000)
      WRITE(6,1010)(X(I),I=1,IMAX)
      WRITE(6, 1100)
 1100 FORMAT(1H0,5%,'J',9%,'Y(J)',15%,'EDENS(I,J),I=1,IMAX',//)
      DO 154 JJ=1, JMAX
      J=JMAX+1-JJ
      DO 152 I=1, IMAX
  152 SCRTCH(I)=EDENS(I,J)*DNSNRM
```

WRITE(6,1030)J,Y(J),(SCRTCH(I),I=1,10)

```
WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
 154 CONTINUE
     WRITE(6, 1000)
     WRITE(6,1010)(X(I), I=1, IMAX)
     WRITE(6, 1070)
1070 FORMAT(1H0.5X,'J'.9X,'Y(J)',15X,'ESUBX(I,J),I=1,IMAX',//)
    DO 170 JJ=1. JMAX
     J=JMAX+1-JJ
     DO 160 I=1. IMAX
160 SCRTCH(I)=ESUBX(I,J)*PSINRM/DSTNRM
     WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
     WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
 170 CONTINUE
    WRITE(6, 1000)
    WRITE(6,1010)(X(I),I=1,IMAX)
     WRITE(6, 1080)
1080 FORMAT(1H0,5X,'J',9X,'Y(J)',15X,'ESUBY(I,J),I=1,IMAX',//)
    DO 190 JJ=1, JMAX
     J=JMAX+1-JJ
    DO 180 I=1, IMAX
180 SCRICH(I)=ESUBY(I,J)*PSINRM/DSTNRM
    WRITE(6,1030) J.Y(J),(SCRTCH(I), I=1,10)
    WRITE(6,1040)(SCRTCH(I), I=11, IMAX)
190 CONTINUE
    WRITE(6,1000)
    WRITE(6,1010)(X(I),I=1,IMAX)
    WRITE(6, 1090)
1090 FORMAT(1H0,5%,'J',9%,'Y(J)',15%,'ETOTAL(I,J),I=1,IMAX',//)
    00 210 JJ=1, JMAX
     J=JMAX+1-JJ
    DO 200 I=1, IMAX
200 SCRTCH(I)=SQRT(ESUBX(I,J)*ESUBX(I,J)+ESUBY(I,J)*ESUBY(I,J))*
    &PSIHRM/DSTNRM
    WRITE(6,1030) J,Y(J),(SCRTCH(I),I=1,10)
    WRITHEC 6, 1043 XCBORTOHCI), I=11, IMAK)
210 CONTINUE
    RETURN
    END
```

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